



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 17, 2019 – 11:16 AM EDT

PDB ID : 6JSH  
EMDB ID: : EMD-9881  
Title : Apo-state Fatty Acid Synthase  
Authors : Qiu, S.W.; Liu, S.  
Deposited on : 2019-04-08  
Resolution : 5.10 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

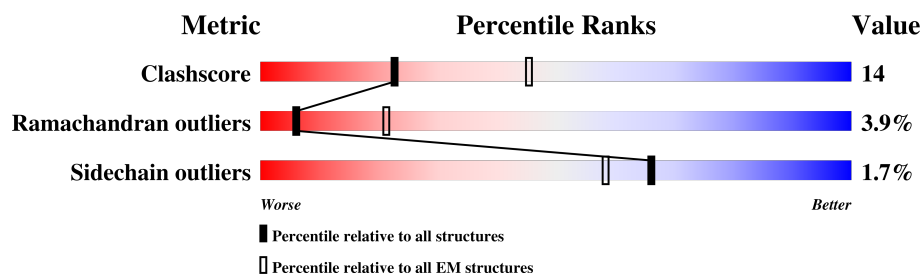
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	2051	70% 22% • 7%
1	F	2051	70% 22% • 7%
1	G	2051	70% 22% • 7%
2	A	1887	36% 16% • 46%
2	D	1887	36% 16% • 46%
2	E	1887	36% 16% • 46%
3	C	71	65% 34% •
3	H	71	66% 32% •
3	I	71	68% 31% •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58170 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	F	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	G	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		

- Molecule 2 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1011	Total	C	N	O	S	0	0
			7037	4419	1224	1363	31		
2	D	1011	Total	C	N	O	S	0	0
			7037	4419	1224	1363	31		
2	E	1011	Total	C	N	O	S	0	0
			7037	4419	1224	1363	31		

- Molecule 3 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	H	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	I	71	Total	C	N	O	S	0	0
			607	376	109	121	1		

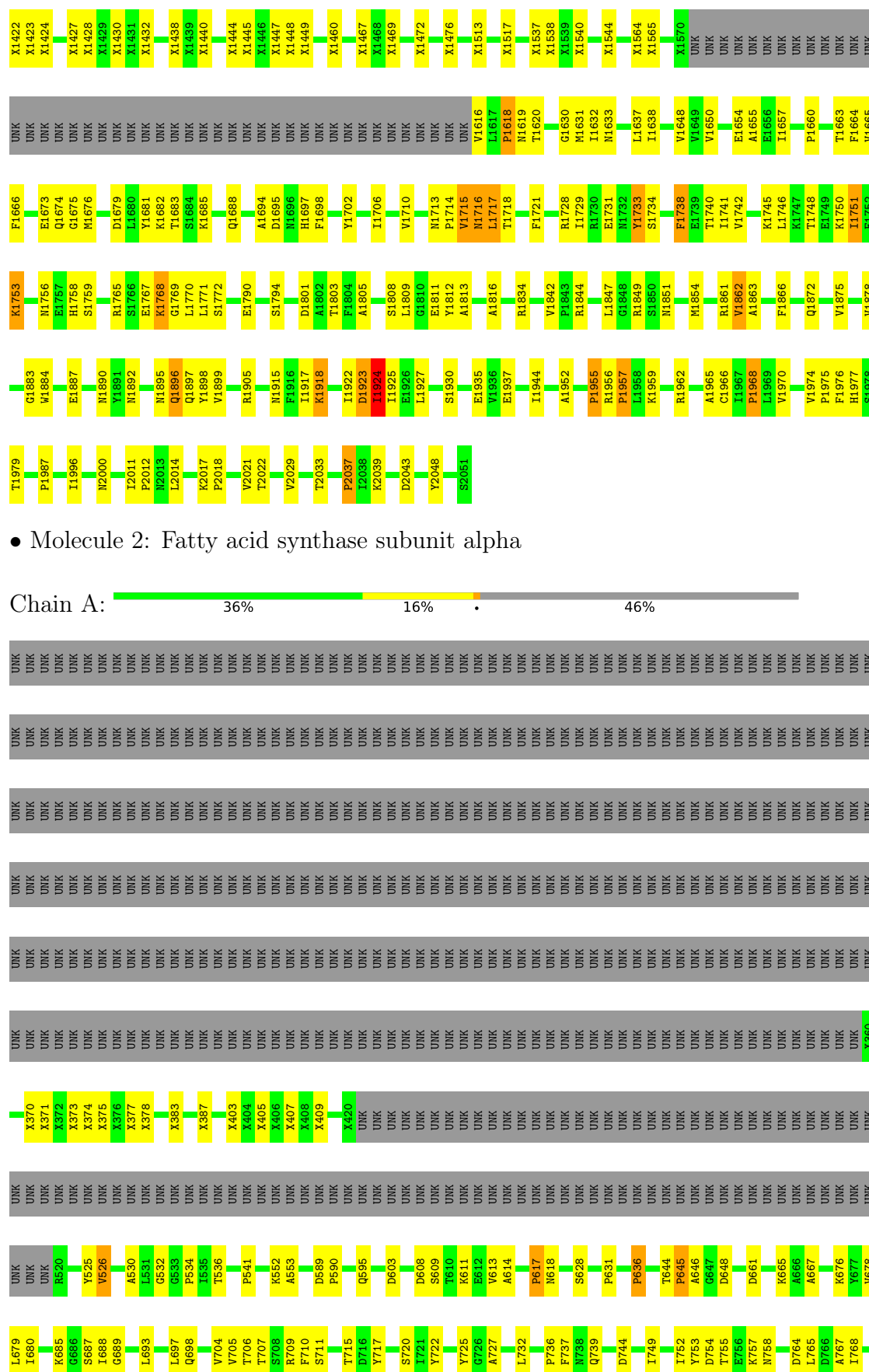






Device Type	Percentage
Smartphone	70%
Tablet	22%
Feature phone	7%

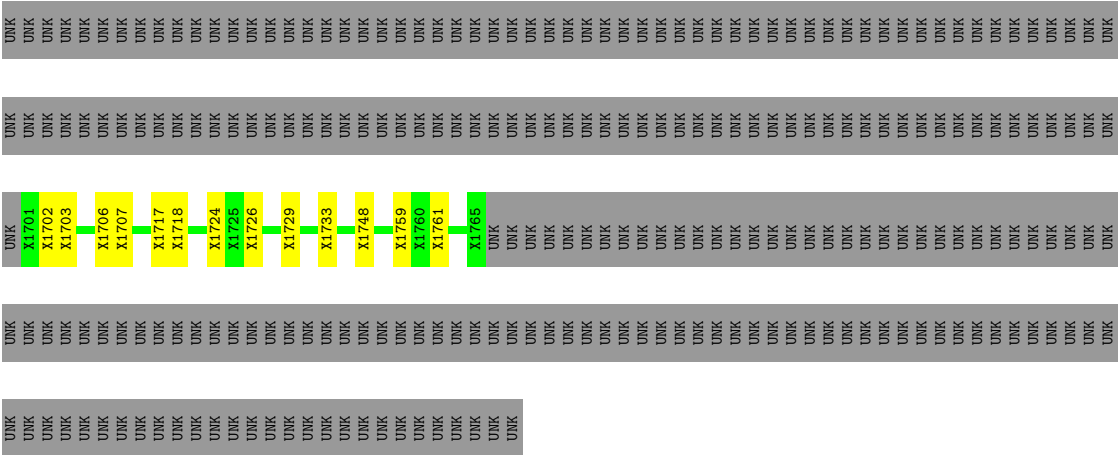




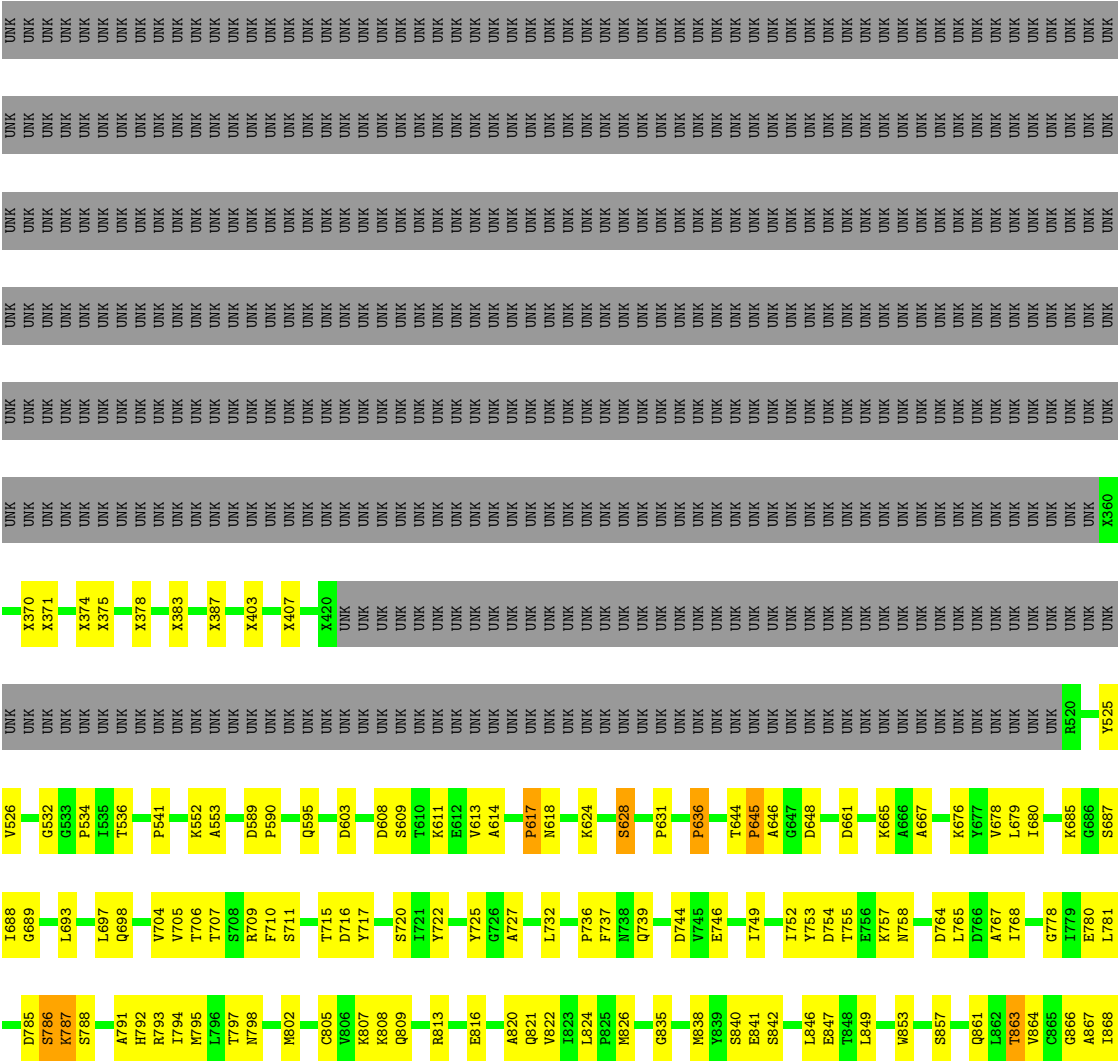
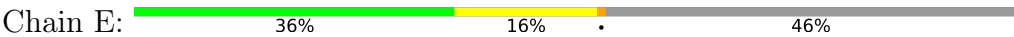


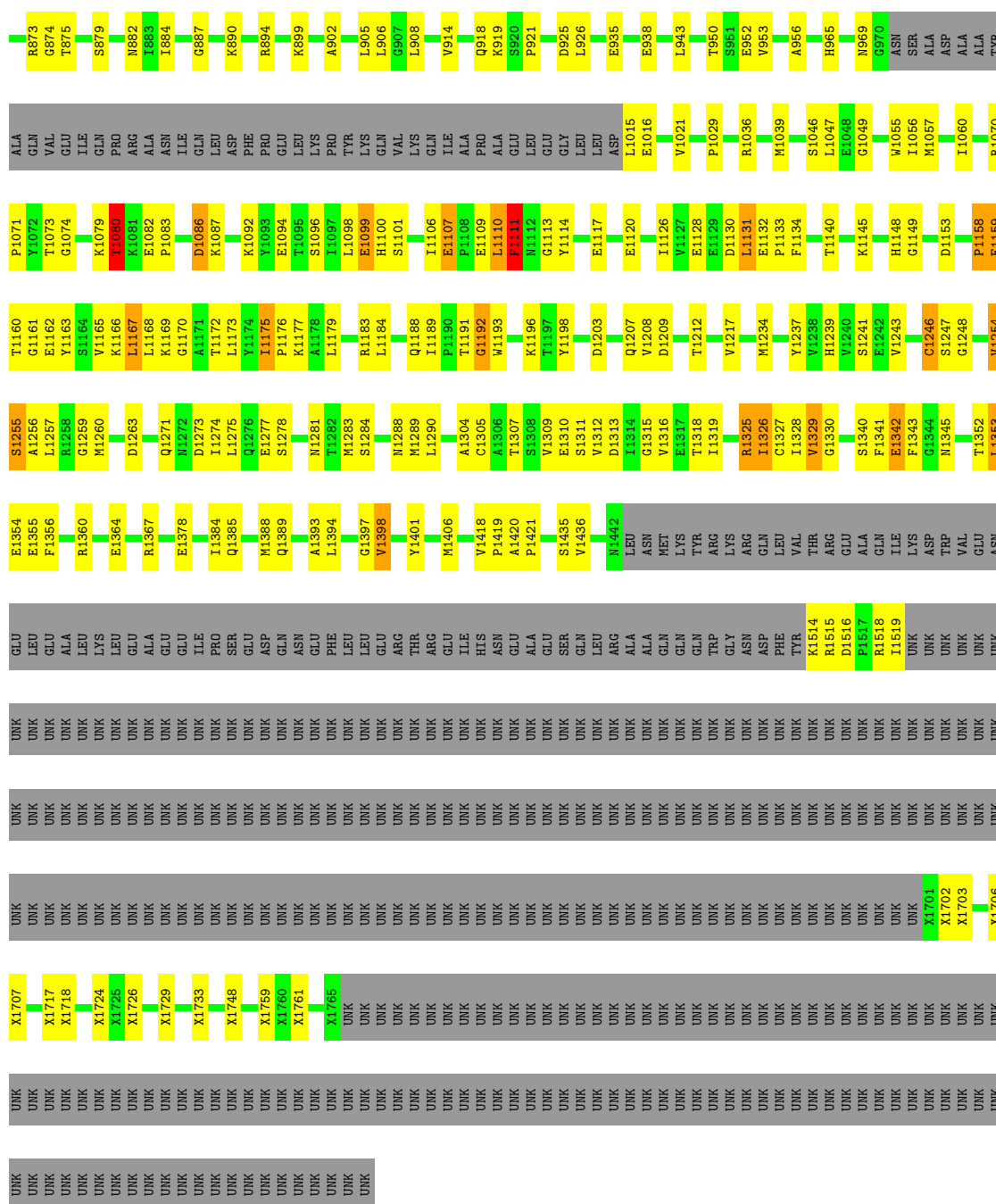




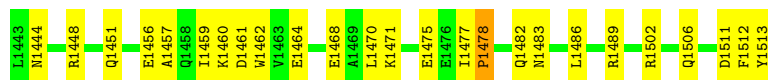
● Molecule 2: Fatty acid synthase subunit alpha





• Molecule 3: Fatty acid synthase subunit alpha

Chain C: 65% 34%



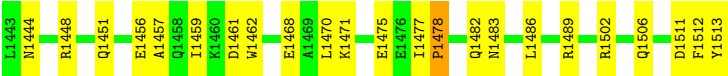
• Molecule 3: Fatty acid synthase subunit alpha

Chain H: 66% 32%



- Molecule 3: Fatty acid synthase subunit alpha

Chain I:  68%  31% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	11608	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.278	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	B	0.41	0/7308	0.73	17/9952 (0.2%)
1	F	0.41	0/7308	0.73	17/9952 (0.2%)
1	G	0.41	0/7308	0.73	17/9952 (0.2%)
2	A	0.47	0/6518	0.80	12/8839 (0.1%)
2	D	0.47	0/6518	0.80	12/8839 (0.1%)
2	E	0.47	0/6518	0.80	12/8839 (0.1%)
3	C	0.40	0/616	0.69	0/828
3	H	0.40	0/616	0.69	0/828
3	I	0.40	0/616	0.69	0/828
All	All	0.44	0/43326	0.76	87/58857 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	15
1	F	0	15
1	G	0	15
2	A	0	25
2	D	0	25
2	E	0	25
3	C	0	2
3	H	0	2
3	I	0	2
All	All	0	126

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1203	ASP	CB-CG-OD1	10.10	127.39	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1203	ASP	CB-CG-OD1	10.09	127.39	118.30
2	E	1203	ASP	CB-CG-OD1	10.06	127.35	118.30
1	G	559	PRO	N-CA-CB	6.80	111.47	103.30
1	B	559	PRO	N-CA-CB	6.80	111.46	103.30
1	F	559	PRO	N-CA-CB	6.79	111.45	103.30
1	F	1957	PRO	N-CA-CB	6.75	111.39	103.30
1	G	1957	PRO	N-CA-CB	6.74	111.38	103.30
1	B	1957	PRO	N-CA-CB	6.69	111.33	103.30
1	B	1955	PRO	N-CA-CB	6.64	111.27	103.30
1	G	1955	PRO	N-CA-CB	6.64	111.27	103.30
1	F	1955	PRO	N-CA-CB	6.64	111.26	103.30
1	F	1975	PRO	N-CA-CB	6.63	111.26	103.30
1	G	1975	PRO	N-CA-CB	6.59	111.20	103.30
1	B	1975	PRO	N-CA-CB	6.58	111.20	103.30
1	F	1987	PRO	N-CA-CB	6.54	111.15	103.30
1	G	1987	PRO	N-CA-CB	6.51	111.11	103.30
1	B	1987	PRO	N-CA-CB	6.50	111.09	103.30
1	B	2012	PRO	N-CA-CB	6.42	111.00	103.30
2	D	636	PRO	N-CA-CB	6.42	111.01	103.30
1	F	2012	PRO	N-CA-CB	6.41	111.00	103.30
1	G	2012	PRO	N-CA-CB	6.41	110.99	103.30
2	A	636	PRO	N-CA-CB	6.41	110.99	103.30
1	G	2037	PRO	N-CA-CB	6.40	110.98	103.30
2	E	636	PRO	N-CA-CB	6.38	110.95	103.30
1	B	2037	PRO	N-CA-CB	6.37	110.95	103.30
1	F	2037	PRO	N-CA-CB	6.36	110.93	103.30
2	D	534	PRO	N-CA-CB	6.35	110.92	103.30
1	F	567	PRO	N-CA-CB	6.34	110.90	103.30
2	E	534	PRO	N-CA-CB	6.32	110.88	103.30
2	E	1173	LEU	CA-CB-CG	6.32	129.83	115.30
1	B	567	PRO	N-CA-CB	6.31	110.88	103.30
2	A	534	PRO	N-CA-CB	6.30	110.86	103.30
1	G	567	PRO	N-CA-CB	6.30	110.86	103.30
1	B	1968	PRO	N-CA-CB	6.30	110.86	103.30
2	D	1173	LEU	CA-CB-CG	6.30	129.79	115.30
1	F	1968	PRO	N-CA-CB	6.30	110.86	103.30
2	A	1173	LEU	CA-CB-CG	6.29	129.78	115.30
1	F	1660	PRO	N-CA-CB	6.28	110.83	103.30
1	G	1660	PRO	N-CA-CB	6.25	110.79	103.30
1	G	1968	PRO	N-CA-CB	6.25	110.79	103.30
1	B	1660	PRO	N-CA-CB	6.24	110.78	103.30
1	B	1717	LEU	CA-CB-CG	6.11	129.36	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1717	LEU	CA-CB-CG	6.11	129.35	115.30
1	G	1717	LEU	CA-CB-CG	6.10	129.33	115.30
2	D	541	PRO	N-CA-CB	6.02	110.53	103.30
2	E	1131	LEU	CA-CB-CG	6.02	129.15	115.30
2	D	1131	LEU	CA-CB-CG	6.02	129.14	115.30
2	A	1131	LEU	CA-CB-CG	6.00	129.10	115.30
2	A	541	PRO	N-CA-CB	5.96	110.45	103.30
2	E	541	PRO	N-CA-CB	5.95	110.44	103.30
2	E	617	PRO	N-CA-CB	5.81	110.27	103.30
2	D	617	PRO	N-CA-CB	5.79	110.25	103.30
1	G	1738	PHE	CB-CG-CD1	5.76	124.83	120.80
2	A	617	PRO	N-CA-CB	5.76	110.21	103.30
1	B	1618	PRO	N-CA-CB	5.74	110.19	103.30
1	B	1738	PHE	CB-CG-CD1	5.74	124.81	120.80
1	F	1618	PRO	N-CA-CB	5.72	110.16	103.30
2	E	590	PRO	N-CA-CB	5.71	110.15	103.30
1	F	1738	PHE	CB-CG-CD1	5.70	124.79	120.80
1	G	1618	PRO	N-CA-CB	5.70	110.14	103.30
2	A	590	PRO	N-CA-CB	5.68	110.11	103.30
2	D	590	PRO	N-CA-CB	5.67	110.10	103.30
1	F	2018	PRO	N-CA-CB	5.62	110.05	103.30
1	B	2018	PRO	N-CA-CB	5.62	110.05	103.30
1	G	2018	PRO	N-CA-CB	5.61	110.03	103.30
2	A	645	PRO	N-CA-CB	5.45	109.84	103.30
2	E	645	PRO	N-CA-CB	5.45	109.83	103.30
2	D	645	PRO	N-CA-CB	5.43	109.82	103.30
1	F	168	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	168	ASP	CB-CG-OD1	5.40	123.16	118.30
2	A	631	PRO	N-CA-CB	5.40	109.78	103.30
2	D	1175	ILE	C-N-CD	-5.40	108.73	120.60
1	G	168	ASP	CB-CG-OD1	5.39	123.16	118.30
2	E	1175	ILE	C-N-CD	-5.38	108.75	120.60
2	A	1175	ILE	C-N-CD	-5.38	108.76	120.60
2	E	631	PRO	N-CA-CB	5.34	109.71	103.30
2	D	631	PRO	N-CA-CB	5.32	109.68	103.30
1	F	1923	ASP	C-N-CA	5.25	134.82	121.70
1	G	1923	ASP	C-N-CA	5.24	134.81	121.70
1	B	1923	ASP	C-N-CA	5.23	134.78	121.70
1	G	533	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	533	LEU	CA-CB-CG	5.09	127.01	115.30
1	F	533	LEU	CA-CB-CG	5.09	127.01	115.30
2	E	1398	VAL	C-N-CD	-5.01	109.57	120.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1398	VAL	C-N-CD	-5.01	109.58	120.60
2	A	1398	VAL	C-N-CD	-5.00	109.60	120.60

There are no chirality outliers.

All (126) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1070	ARG	Peptide
2	A	1080	THR	Peptide
2	A	1082	GLU	Peptide
2	A	1086	ASP	Peptide
2	A	1087	LYS	Peptide
2	A	1099	GLU	Peptide
2	A	1107	GLU	Peptide
2	A	1110	LEU	Peptide
2	A	1111	PHE	Peptide
2	A	1134	PHE	Peptide
2	A	1158	PRO	Peptide
2	A	1167	LEU	Peptide
2	A	1172	THR	Peptide
2	A	1192	GLY	Peptide
2	A	1208	VAL	Peptide
2	A	1209	ASP	Peptide
2	A	1237	TYR	Peptide
2	A	1254	VAL	Peptide
2	A	1325	ARG	Peptide
2	A	1341	PHE	Peptide
2	A	1342	GLU	Peptide
2	A	1353	LEU	Peptide
2	A	1354	GLU	Peptide
2	A	786	SER	Peptide
2	A	894	ARG	Peptide
1	B	1630	GLY	Peptide
1	B	1715	VAL	Peptide
1	B	1733	TYR	Peptide
1	B	1746	LEU	Peptide
1	B	1751	ILE	Peptide
1	B	1847	LEU	Peptide
1	B	1861	ARG	Peptide
1	B	1862	VAL	Peptide
1	B	1896	GLN	Peptide
1	B	1918	LYS	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	1922	ILE	Peptide
1	B	1924	ILE	Peptide
1	B	446	ASN	Peptide
1	B	471	LEU	Peptide
1	B	474	SER	Peptide
3	C	1462	TRP	Peptide
3	C	1477	ILE	Peptide
2	D	1070	ARG	Peptide
2	D	1080	THR	Peptide
2	D	1082	GLU	Peptide
2	D	1086	ASP	Peptide
2	D	1087	LYS	Peptide
2	D	1099	GLU	Peptide
2	D	1107	GLU	Peptide
2	D	1110	LEU	Peptide
2	D	1111	PHE	Peptide
2	D	1134	PHE	Peptide
2	D	1158	PRO	Peptide
2	D	1167	LEU	Peptide
2	D	1172	THR	Peptide
2	D	1192	GLY	Peptide
2	D	1208	VAL	Peptide
2	D	1209	ASP	Peptide
2	D	1237	TYR	Peptide
2	D	1254	VAL	Peptide
2	D	1325	ARG	Peptide
2	D	1341	PHE	Peptide
2	D	1342	GLU	Peptide
2	D	1353	LEU	Peptide
2	D	1354	GLU	Peptide
2	D	786	SER	Peptide
2	D	894	ARG	Peptide
2	E	1070	ARG	Peptide
2	E	1080	THR	Peptide
2	E	1082	GLU	Peptide
2	E	1086	ASP	Peptide
2	E	1087	LYS	Peptide
2	E	1099	GLU	Peptide
2	E	1107	GLU	Peptide
2	E	1110	LEU	Peptide
2	E	1111	PHE	Peptide
2	E	1134	PHE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	E	1158	PRO	Peptide
2	E	1167	LEU	Peptide
2	E	1172	THR	Peptide
2	E	1192	GLY	Peptide
2	E	1208	VAL	Peptide
2	E	1209	ASP	Peptide
2	E	1237	TYR	Peptide
2	E	1254	VAL	Peptide
2	E	1325	ARG	Peptide
2	E	1341	PHE	Peptide
2	E	1342	GLU	Peptide
2	E	1353	LEU	Peptide
2	E	1354	GLU	Peptide
2	E	786	SER	Peptide
2	E	894	ARG	Peptide
1	F	1630	GLY	Peptide
1	F	1715	VAL	Peptide
1	F	1733	TYR	Peptide
1	F	1746	LEU	Peptide
1	F	1751	ILE	Peptide
1	F	1847	LEU	Peptide
1	F	1861	ARG	Peptide
1	F	1862	VAL	Peptide
1	F	1896	GLN	Peptide
1	F	1918	LYS	Peptide
1	F	1922	ILE	Peptide
1	F	1924	ILE	Peptide
1	F	446	ASN	Peptide
1	F	471	LEU	Peptide
1	F	474	SER	Peptide
1	G	1630	GLY	Peptide
1	G	1715	VAL	Peptide
1	G	1733	TYR	Peptide
1	G	1746	LEU	Peptide
1	G	1751	ILE	Peptide
1	G	1847	LEU	Peptide
1	G	1861	ARG	Peptide
1	G	1862	VAL	Peptide
1	G	1896	GLN	Peptide
1	G	1918	LYS	Peptide
1	G	1922	ILE	Peptide
1	G	1924	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	G	446	ASN	Peptide
1	G	471	LEU	Peptide
1	G	474	SER	Peptide
3	H	1462	TRP	Peptide
3	H	1477	ILE	Peptide
3	I	1462	TRP	Peptide
3	I	1477	ILE	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	11746	0	7719	272	0
1	F	11746	0	7719	263	0
1	G	11746	0	7720	272	0
2	A	7037	0	6113	180	0
2	D	7037	0	6113	177	0
2	E	7037	0	6113	181	0
3	C	607	0	580	14	0
3	H	607	0	580	12	0
3	I	607	0	580	12	0
All	All	58170	0	43237	1374	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1374) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:678:VAL:HG12	2:E:767:ALA:HB3	1.69	0.74
1:B:520:LYS:HB2	1:B:526:ARG:HH22	1.53	0.74
1:F:520:LYS:HB2	1:F:526:ARG:HH22	1.53	0.73
1:G:520:LYS:HB2	1:G:526:ARG:HH22	1.53	0.73
2:D:678:VAL:HG12	2:D:767:ALA:HB3	1.69	0.73
2:D:1340:SER:HA	2:D:1343:PHE:HB2	1.71	0.73
2:A:678:VAL:HG12	2:A:767:ALA:HB3	1.69	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1340:SER:HA	2:E:1343:PHE:HB2	1.71	0.72
2:A:1340:SER:HA	2:A:1343:PHE:HB2	1.71	0.71
2:A:1254:VAL:HG23	2:A:1257:LEU:HB3	1.73	0.71
1:B:453:LYS:HG3	1:B:469:ARG:HE	1.56	0.70
1:F:453:LYS:HG3	1:F:469:ARG:HE	1.56	0.69
1:B:234:ILE:HD13	1:B:425:SER:HB2	1.75	0.69
2:D:1254:VAL:HG23	2:D:1257:LEU:HB3	1.73	0.69
1:F:1565:UNK:H	1:F:1654:GLU:HA	1.58	0.69
1:G:234:ILE:HD13	1:G:425:SER:HB2	1.75	0.69
1:G:453:LYS:HG3	1:G:469:ARG:HE	1.56	0.69
2:E:1254:VAL:HG23	2:E:1257:LEU:HB3	1.73	0.68
1:B:1834:ARG:HH21	1:B:2048:TYR:HA	1.58	0.68
1:F:1834:ARG:HH21	1:F:2048:TYR:HA	1.58	0.68
1:F:234:ILE:HD13	1:F:425:SER:HB2	1.75	0.68
1:F:397:LYS:HZ1	1:F:416:PHE:HB2	1.57	0.68
1:G:1565:UNK:H	1:G:1654:GLU:HA	1.58	0.68
1:G:1834:ARG:HH21	1:G:2048:TYR:HA	1.58	0.68
1:B:1565:UNK:H	1:B:1654:GLU:HA	1.58	0.68
1:G:53:GLU:HG3	1:G:55:THR:H	1.60	0.66
2:D:1319:ILE:HD13	2:D:1325:ARG:HA	1.78	0.65
1:F:53:GLU:HG3	1:F:55:THR:H	1.60	0.65
1:B:826:UNK:HA	1:B:835:UNK:HA	1.78	0.65
1:B:53:GLU:HG3	1:B:55:THR:H	1.60	0.65
1:G:397:LYS:HZ1	1:G:416:PHE:HB2	1.61	0.65
2:A:1319:ILE:HD13	2:A:1325:ARG:HA	1.78	0.65
2:A:1329:VAL:HG12	2:A:1384:ILE:HD12	1.79	0.65
2:E:1329:VAL:HG12	2:E:1384:ILE:HD12	1.79	0.65
1:B:387:TYR:HA	1:B:390:ASN:HD22	1.62	0.65
2:E:785:ASP:OD1	2:E:785:ASP:N	2.30	0.64
1:F:387:TYR:HA	1:F:390:ASN:HD22	1.62	0.64
2:A:785:ASP:N	2:A:785:ASP:OD1	2.30	0.64
1:F:826:UNK:HA	1:F:835:UNK:HA	1.78	0.64
2:A:1159:GLU:HB2	2:A:1167:LEU:HB3	1.80	0.64
1:G:826:UNK:HA	1:G:835:UNK:HA	1.78	0.63
2:E:1159:GLU:HB2	2:E:1167:LEU:HB3	1.80	0.63
2:E:1319:ILE:HD13	2:E:1325:ARG:HA	1.78	0.63
1:G:387:TYR:HA	1:G:390:ASN:HD22	1.62	0.63
2:D:785:ASP:N	2:D:785:ASP:OD1	2.31	0.63
1:G:157:VAL:HG13	1:G:269:GLY:HA3	1.81	0.63
2:D:1329:VAL:HG12	2:D:1384:ILE:HD12	1.79	0.63
1:B:397:LYS:HZ1	1:B:416:PHE:HB2	1.64	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1345:UNK:HA	1:F:1363:UNK:HA	1.82	0.62
2:D:1356:PHE:O	2:D:1360:ARG:NH1	2.33	0.62
2:E:965:HIS:O	2:E:969:ASN:ND2	2.33	0.62
2:D:1159:GLU:HB2	2:D:1167:LEU:HB3	1.80	0.62
1:F:1808:SER:H	1:F:1811:GLU:HG3	1.65	0.62
1:G:1345:UNK:HA	1:G:1363:UNK:HA	1.81	0.62
2:E:1356:PHE:O	2:E:1360:ARG:NH1	2.33	0.62
1:F:131:ILE:HG13	1:F:182:VAL:HG11	1.82	0.62
1:B:1808:SER:H	1:B:1811:GLU:HG3	1.65	0.61
1:G:131:ILE:HG13	1:G:182:VAL:HG11	1.82	0.61
2:A:965:HIS:O	2:A:969:ASN:ND2	2.33	0.61
1:F:157:VAL:HG13	1:F:269:GLY:HA3	1.81	0.61
2:A:1079:LYS:HE2	2:A:1080:THR:HG22	1.83	0.61
1:B:131:ILE:HG13	1:B:182:VAL:HG11	1.82	0.61
3:C:1468:GLU:HA	3:C:1471:LYS:HB2	1.82	0.61
1:F:78:GLY:HA2	1:F:81:ASP:HB3	1.83	0.61
2:A:1356:PHE:O	2:A:1360:ARG:NH1	2.33	0.61
1:B:157:VAL:HG13	1:B:269:GLY:HA3	1.81	0.61
1:G:78:GLY:HA2	1:G:81:ASP:HB3	1.83	0.61
1:B:1336:UNK:HA	1:B:1379:UNK:HA	1.83	0.61
3:C:1483:ASN:HA	3:C:1486:LEU:HB2	1.81	0.61
2:E:1079:LYS:HE2	2:E:1080:THR:HG22	1.83	0.61
1:F:1336:UNK:HA	1:F:1379:UNK:HA	1.83	0.61
3:H:1483:ASN:HA	3:H:1486:LEU:HB2	1.81	0.61
2:D:1239:HIS:HB2	2:D:1241:SER:H	1.66	0.61
2:E:1239:HIS:HB2	2:E:1241:SER:H	1.66	0.61
2:A:697:LEU:HD22	2:A:732:LEU:HD21	1.82	0.61
2:D:1435:SER:HA	2:D:1518:ARG:HH12	1.66	0.61
3:I:1483:ASN:HA	3:I:1486:LEU:HB2	1.81	0.61
1:B:78:GLY:HA2	1:B:81:ASP:HB3	1.83	0.61
1:G:1336:UNK:HA	1:G:1379:UNK:HA	1.83	0.60
1:B:1345:UNK:HA	1:B:1363:UNK:HA	1.82	0.60
2:E:1435:SER:HA	2:E:1518:ARG:HH12	1.66	0.60
1:G:1808:SER:H	1:G:1811:GLU:HG3	1.65	0.60
2:E:697:LEU:HD22	2:E:732:LEU:HD21	1.82	0.60
3:I:1468:GLU:HA	3:I:1471:LYS:HB2	1.82	0.60
2:A:1435:SER:HA	2:A:1518:ARG:HH12	1.66	0.60
2:D:697:LEU:HD22	2:D:732:LEU:HD21	1.82	0.60
1:G:108:LEU:HD11	1:G:122:LEU:HD12	1.84	0.60
2:D:749:ILE:HD12	2:D:752:ILE:HD11	1.84	0.60
1:F:108:LEU:HD11	1:F:122:LEU:HD12	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:1468:GLU:HA	3:H:1471:LYS:HB2	1.82	0.60
1:B:108:LEU:HD11	1:B:122:LEU:HD12	1.84	0.60
1:B:130:ARG:NH2	1:B:136:PRO:O	2.34	0.60
1:B:338:MET:HG2	1:B:421:LEU:HD13	1.83	0.60
2:D:965:HIS:O	2:D:969:ASN:ND2	2.33	0.60
2:A:1239:HIS:HB2	2:A:1241:SER:H	1.66	0.60
1:F:130:ARG:NH2	1:F:136:PRO:O	2.34	0.60
1:G:130:ARG:NH2	1:G:136:PRO:O	2.34	0.59
1:G:1427:UNK:HA	1:G:1445:UNK:HA	1.84	0.59
2:A:749:ILE:HD12	2:A:752:ILE:HD11	1.84	0.59
2:E:749:ILE:HD12	2:E:752:ILE:HD11	1.84	0.59
1:F:338:MET:HG2	1:F:421:LEU:HD13	1.83	0.59
1:F:234:ILE:HG13	1:F:235:PRO:HD3	1.84	0.59
1:G:338:MET:HG2	1:G:421:LEU:HD13	1.83	0.59
1:B:1391:UNK:HA	1:B:1422:UNK:HA	1.84	0.59
1:F:227:ASP:O	1:F:231:LEU:N	2.36	0.59
1:G:234:ILE:HG13	1:G:235:PRO:HD3	1.84	0.59
2:A:1140:THR:HA	2:A:1165:VAL:HG21	1.85	0.59
1:B:1883:GLY:HA3	1:B:1892:ASN:HB2	1.85	0.59
1:B:234:ILE:HG13	1:B:235:PRO:HD3	1.84	0.59
2:D:1079:LYS:HE2	2:D:1080:THR:HG22	1.83	0.59
2:E:1140:THR:HA	2:E:1165:VAL:HG21	1.85	0.59
1:G:245:GLN:NE2	1:G:279:THR:OG1	2.36	0.59
1:B:1663:THR:O	2:E:1718:UNK:N	2.36	0.59
1:F:168:ASP:OD1	1:F:169:TYR:N	2.36	0.59
2:A:679:LEU:HD13	2:A:704:VAL:HG13	1.84	0.59
1:G:1883:GLY:HA3	1:G:1892:ASN:HB2	1.85	0.59
1:B:1427:UNK:HA	1:B:1445:UNK:HA	1.84	0.58
1:B:168:ASP:OD1	1:B:169:TYR:N	2.36	0.58
2:D:679:LEU:HD13	2:D:704:VAL:HG13	1.84	0.58
2:E:1169:LYS:HZ2	2:E:1170:GLY:H	1.51	0.58
1:F:1427:UNK:HA	1:F:1445:UNK:HA	1.84	0.58
1:B:202:THR:OG1	1:B:309:ARG:NH2	2.37	0.58
2:D:1169:LYS:HZ2	2:D:1170:GLY:H	1.51	0.58
2:E:1036:ARG:HA	2:E:1039:MET:HB2	1.86	0.58
1:G:259:THR:HA	1:G:289:TRP:HE1	1.69	0.58
1:B:1537:UNK:O	1:B:1620:THR:N	2.36	0.58
1:B:259:THR:HA	1:B:289:TRP:HE1	1.69	0.58
1:G:1537:UNK:O	1:G:1620:THR:N	2.36	0.58
1:G:238:CYS:HA	1:G:275:GLN:HE21	1.69	0.58
2:A:1718:UNK:N	1:F:1663:THR:O	2.36	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:679:LEU:HD13	2:E:704:VAL:HG13	1.84	0.58
1:F:1715:VAL:HA	1:F:1769:GLY:HA2	1.85	0.58
1:F:1750:LYS:HB2	1:F:1753:LYS:HE3	1.85	0.58
1:G:202:THR:OG1	1:G:309:ARG:NH2	2.37	0.58
1:B:1447:UNK:N	1:B:1460:UNK:O	2.36	0.58
2:D:1140:THR:HA	2:D:1165:VAL:HG21	1.85	0.58
1:F:1391:UNK:HA	1:F:1422:UNK:HA	1.84	0.58
1:F:245:GLN:NE2	1:F:279:THR:OG1	2.36	0.58
1:G:168:ASP:OD1	1:G:169:TYR:N	2.36	0.58
1:B:238:CYS:HA	1:B:275:GLN:HE21	1.69	0.58
1:F:1447:UNK:N	1:F:1460:UNK:O	2.36	0.58
1:F:1537:UNK:O	1:F:1620:THR:N	2.36	0.58
2:D:1718:UNK:N	1:G:1663:THR:O	2.37	0.58
2:A:1161:GLY:H	2:A:1166:LYS:HA	1.69	0.58
1:B:245:GLN:NE2	1:B:279:THR:OG1	2.36	0.58
2:D:1161:GLY:H	2:D:1166:LYS:HA	1.69	0.58
1:G:1715:VAL:HA	1:G:1769:GLY:HA2	1.85	0.58
1:G:1750:LYS:HB2	1:G:1753:LYS:HE3	1.85	0.58
1:B:727:UNK:O	1:B:835:UNK:N	2.37	0.58
1:F:727:UNK:O	1:F:835:UNK:N	2.37	0.58
2:A:1243:VAL:HG21	2:A:1325:ARG:HG3	1.85	0.58
1:B:1513:UNK:O	1:B:1517:UNK:N	2.37	0.58
1:B:1540:UNK:O	1:B:1544:UNK:N	2.37	0.58
1:B:527:VAL:HG13	1:B:541:TYR:HA	1.86	0.58
1:F:1884:TRP:O	1:F:1892:ASN:ND2	2.37	0.58
1:F:259:THR:HA	1:F:289:TRP:HE1	1.69	0.58
1:F:527:VAL:HG13	1:F:541:TYR:HA	1.86	0.58
1:G:727:UNK:O	1:G:835:UNK:N	2.37	0.58
2:A:1169:LYS:HZ2	2:A:1170:GLY:H	1.51	0.58
1:F:1883:GLY:HA3	1:F:1892:ASN:HB2	1.85	0.58
1:F:202:THR:OG1	1:F:309:ARG:NH2	2.37	0.58
1:G:1391:UNK:HA	1:G:1422:UNK:HA	1.84	0.58
1:B:1728:ARG:NH1	1:B:1731:GLU:OE1	2.36	0.57
1:B:1750:LYS:HB2	1:B:1753:LYS:HE3	1.85	0.57
1:B:1884:TRP:O	1:B:1892:ASN:ND2	2.37	0.57
1:G:1447:UNK:N	1:G:1460:UNK:O	2.36	0.57
1:B:229:ASP:N	1:B:229:ASP:OD1	2.37	0.57
2:E:1243:VAL:HG21	2:E:1325:ARG:HG3	1.85	0.57
1:F:238:CYS:HA	1:F:275:GLN:HE21	1.68	0.57
1:G:405:SER:O	1:G:406:ARG:NH1	2.37	0.57
1:B:1715:VAL:HA	1:B:1769:GLY:HA2	1.85	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:952:GLU:O	2:E:956:ALA:N	2.37	0.57
2:A:1036:ARG:HA	2:A:1039:MET:HB2	1.85	0.57
2:A:952:GLU:O	2:A:956:ALA:N	2.37	0.57
2:D:1243:VAL:HG21	2:D:1325:ARG:HG3	1.85	0.57
1:G:1884:TRP:O	1:G:1892:ASN:ND2	2.37	0.57
1:G:53:GLU:OE2	1:G:55:THR:OG1	2.23	0.57
2:E:1106:ILE:HG23	2:E:1192:GLY:HA2	1.87	0.57
1:G:1540:UNK:O	1:G:1544:UNK:N	2.37	0.57
1:G:1679:ASP:N	1:G:1679:ASP:OD2	2.38	0.57
2:E:786:SER:O	2:E:788:SER:N	2.38	0.57
1:G:1513:UNK:O	1:G:1517:UNK:N	2.37	0.57
1:G:527:VAL:HG13	1:G:541:TYR:HA	1.86	0.57
2:A:1120:GLU:O	2:A:1183:ARG:NH2	2.38	0.57
2:A:786:SER:O	2:A:788:SER:N	2.38	0.57
1:B:227:ASP:O	1:B:231:LEU:N	2.36	0.57
2:D:1036:ARG:HA	2:D:1039:MET:HB2	1.86	0.57
2:A:864:VAL:HG13	2:A:921:PRO:HB3	1.86	0.56
2:E:1130:ASP:OD1	2:E:1130:ASP:N	2.38	0.56
2:E:1161:GLY:H	2:E:1166:LYS:HA	1.69	0.56
1:F:1679:ASP:OD2	1:F:1679:ASP:N	2.38	0.56
1:G:1728:ARG:NH1	1:G:1731:GLU:OE1	2.36	0.56
1:B:428:HIS:H	1:B:484:ILE:HG22	1.70	0.56
2:D:1130:ASP:OD1	2:D:1130:ASP:N	2.38	0.56
1:F:1540:UNK:O	1:F:1544:UNK:N	2.37	0.56
1:G:227:ASP:O	1:G:231:LEU:N	2.36	0.56
2:E:744:ASP:OD1	2:E:744:ASP:N	2.37	0.56
2:E:864:VAL:HG13	2:E:921:PRO:HB3	1.86	0.56
2:D:1106:ILE:HG23	2:D:1192:GLY:HA2	1.86	0.56
2:E:1021:VAL:HG13	2:E:1401:TYR:HB2	1.87	0.56
1:G:428:HIS:H	1:G:484:ILE:HG22	1.70	0.56
1:B:101:ILE:O	1:B:105:ALA:N	2.39	0.56
2:D:786:SER:O	2:D:788:SER:N	2.38	0.56
1:G:268:LYS:NZ	1:G:497:LYS:O	2.36	0.56
2:A:1352:THR:HA	2:A:1355:GLU:HB3	1.88	0.56
2:A:744:ASP:N	2:A:744:ASP:OD1	2.37	0.56
1:F:101:ILE:O	1:F:105:ALA:N	2.39	0.56
1:B:53:GLU:OE2	1:B:55:THR:OG1	2.23	0.56
2:E:709:ARG:NH2	2:E:710:PHE:O	2.39	0.56
1:F:1728:ARG:NH1	1:F:1731:GLU:OE1	2.36	0.56
1:F:346:GLN:HG3	1:F:377:LEU:HD11	1.87	0.56
2:A:1130:ASP:N	2:A:1130:ASP:OD1	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1120:GLU:O	2:D:1183:ARG:NH2	2.38	0.56
2:D:824:LEU:HB3	2:D:846:LEU:HD23	1.88	0.56
2:E:807:LYS:NZ	2:E:816:GLU:OE2	2.39	0.56
1:G:1718:THR:HB	1:G:1770:LEU:HD22	1.87	0.56
2:A:1106:ILE:HG23	2:A:1192:GLY:HA2	1.86	0.56
2:D:864:VAL:HG13	2:D:921:PRO:HB3	1.86	0.56
2:E:1352:THR:HA	2:E:1355:GLU:HB3	1.88	0.56
1:F:1513:UNK:O	1:F:1517:UNK:N	2.37	0.56
2:E:698:GLN:HA	2:E:727:ALA:HB2	1.88	0.56
2:A:1021:VAL:HG13	2:A:1401:TYR:HB2	1.87	0.56
1:B:346:GLN:HG3	1:B:377:LEU:HD11	1.87	0.56
2:D:709:ARG:NH2	2:D:710:PHE:O	2.39	0.56
1:B:288:SER:OG	1:B:289:TRP:N	2.39	0.55
2:D:952:GLU:O	2:D:956:ALA:N	2.37	0.55
2:E:1120:GLU:O	2:E:1183:ARG:NH2	2.38	0.55
2:E:689:GLY:O	2:E:693:LEU:N	2.39	0.55
1:F:229:ASP:OD1	1:F:229:ASP:N	2.37	0.55
1:F:428:HIS:H	1:F:484:ILE:HG22	1.70	0.55
1:G:1538:UNK:O	1:G:1619:ASN:N	2.40	0.55
2:A:709:ARG:NH2	2:A:710:PHE:O	2.39	0.55
2:D:1196:LYS:NZ	2:D:1198:TYR:OH	2.40	0.55
1:F:352:TYR:HA	1:F:355:LYS:HD2	1.89	0.55
1:F:53:GLU:OE2	1:F:55:THR:OG1	2.23	0.55
1:B:405:SER:O	1:B:406:ARG:NH1	2.37	0.55
2:D:1021:VAL:HG13	2:D:1401:TYR:HB2	1.87	0.55
1:G:101:ILE:O	1:G:105:ALA:N	2.39	0.55
1:F:1769:GLY:O	1:F:1772:SER:OG	2.23	0.55
1:B:1718:THR:HB	1:B:1770:LEU:HD22	1.87	0.55
2:D:698:GLN:HA	2:D:727:ALA:HB2	1.88	0.55
2:E:1315:GLY:O	2:E:1318:THR:OG1	2.25	0.55
1:F:1718:THR:HB	1:F:1770:LEU:HD22	1.87	0.55
1:B:1679:ASP:O	1:B:1683:THR:OG1	2.24	0.55
1:B:827:UNK:N	1:B:834:UNK:O	2.40	0.55
1:F:1538:UNK:O	1:F:1619:ASN:N	2.40	0.55
2:A:824:LEU:HB3	2:A:846:LEU:HD23	1.88	0.55
1:F:288:SER:OG	1:F:289:TRP:N	2.39	0.55
1:G:156:LEU:O	1:G:268:LYS:N	2.40	0.55
1:B:1538:UNK:O	1:B:1619:ASN:N	2.40	0.55
2:E:1304:ALA:HA	2:E:1307:THR:HB	1.89	0.55
1:F:827:UNK:N	1:F:834:UNK:O	2.40	0.55
1:G:229:ASP:OD1	1:G:229:ASP:N	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:GLN:HG3	1:G:377:LEU:HD11	1.87	0.54
2:A:1315:GLY:O	2:A:1318:THR:OG1	2.25	0.54
2:A:717:TYR:O	2:A:720:SER:OG	2.26	0.54
1:F:234:ILE:HG23	1:F:424:ALA:HB3	1.88	0.54
1:F:490:TRP:HE1	1:F:516:THR:HG22	1.72	0.54
1:F:847:UNK:O	1:F:851:UNK:N	2.40	0.54
1:G:288:SER:N	1:G:291:SER:OG	2.39	0.54
2:A:824:LEU:O	2:A:867:ALA:N	2.39	0.54
1:B:1694:ALA:HA	1:B:1697:HIS:HB3	1.90	0.54
2:D:717:TYR:O	2:D:720:SER:OG	2.26	0.54
1:F:1147:UNK:O	1:F:1158:UNK:N	2.41	0.54
1:G:1801:ASP:OD1	1:G:1801:ASP:N	2.40	0.54
2:D:1304:ALA:HA	2:D:1307:THR:HB	1.89	0.54
2:E:680:ILE:HB	2:E:705:VAL:HG23	1.90	0.54
1:G:234:ILE:HG23	1:G:424:ALA:HB3	1.88	0.54
1:G:248:HIS:O	1:G:252:THR:OG1	2.25	0.54
1:G:490:TRP:HE1	1:G:516:THR:HG22	1.73	0.54
1:G:847:UNK:O	1:G:851:UNK:N	2.40	0.54
1:B:1698:PHE:O	1:B:1702:TYR:N	2.36	0.54
1:B:288:SER:N	1:B:291:SER:OG	2.39	0.54
2:D:1352:THR:HA	2:D:1355:GLU:HB3	1.88	0.54
1:F:405:SER:O	1:F:406:ARG:NH1	2.37	0.54
1:G:827:UNK:N	1:G:834:UNK:O	2.40	0.54
2:A:698:GLN:HA	2:A:727:ALA:HB2	1.88	0.54
2:D:680:ILE:HB	2:D:705:VAL:HG23	1.89	0.54
1:G:288:SER:OG	1:G:289:TRP:N	2.39	0.54
1:B:847:UNK:O	1:B:851:UNK:N	2.40	0.54
2:D:1717:UNK:O	2:D:1748:UNK:N	2.41	0.54
2:E:798:ASN:O	2:E:802:MET:N	2.41	0.54
2:E:824:LEU:HB3	2:E:846:LEU:HD23	1.88	0.54
1:G:1694:ALA:HA	1:G:1697:HIS:HB3	1.90	0.54
1:G:1769:GLY:O	1:G:1772:SER:OG	2.23	0.54
1:B:1721:PHE:O	1:B:1733:TYR:OH	2.25	0.54
1:B:490:TRP:HE1	1:B:516:THR:HG22	1.73	0.54
2:E:1046:SER:O	2:E:1049:GLY:N	2.31	0.54
2:E:1717:UNK:O	2:E:1748:UNK:N	2.41	0.54
2:E:717:TYR:O	2:E:720:SER:OG	2.26	0.54
1:G:1679:ASP:O	1:G:1683:THR:OG1	2.24	0.54
2:A:798:ASN:O	2:A:802:MET:N	2.41	0.54
1:B:729:UNK:N	1:B:833:UNK:O	2.41	0.54
1:F:288:SER:N	1:F:291:SER:OG	2.39	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1029:PRO:O	2:A:1193:TRP:NE1	2.41	0.54
2:A:1304:ALA:HA	2:A:1307:THR:HB	1.89	0.54
2:D:798:ASN:O	2:D:802:MET:N	2.41	0.54
1:F:729:UNK:N	1:F:833:UNK:O	2.41	0.54
3:H:1470:LEU:HD12	3:H:1489:ARG:HD2	1.90	0.54
2:A:1110:LEU:HB3	2:A:1188:GLN:HA	1.90	0.53
1:F:1729:ILE:O	1:F:1733:TYR:N	2.41	0.53
1:G:1790:GLU:O	1:G:1794:SER:N	2.41	0.53
2:A:1717:UNK:O	2:A:1748:UNK:N	2.41	0.53
1:B:1147:UNK:O	1:B:1158:UNK:N	2.41	0.53
1:B:234:ILE:HG23	1:B:424:ALA:HB3	1.88	0.53
1:B:361:PRO:HD2	1:B:364:LYS:HB2	1.90	0.53
2:E:1109:GLU:H	2:E:1188:GLN:HB2	1.74	0.53
1:F:1679:ASP:O	1:F:1683:THR:OG1	2.24	0.53
1:F:451:ASN:O	1:F:469:ARG:NH1	2.41	0.53
1:G:1721:PHE:O	1:G:1733:TYR:OH	2.25	0.53
3:C:1470:LEU:HD12	3:C:1489:ARG:HD2	1.90	0.53
1:F:6:THR:O	1:F:7:ARG:NH1	2.37	0.53
1:G:1147:UNK:O	1:G:1158:UNK:N	2.41	0.53
2:A:1109:GLU:H	2:A:1188:GLN:HB2	1.74	0.53
2:A:680:ILE:HB	2:A:705:VAL:HG23	1.90	0.53
1:B:122:LEU:HA	1:B:125:ASN:HB2	1.91	0.53
2:D:1046:SER:O	2:D:1049:GLY:N	2.31	0.53
2:D:849:LEU:O	2:D:853:TRP:N	2.42	0.53
1:F:1740:THR:HB	1:F:1751:ILE:HD12	1.91	0.53
1:G:1729:ILE:O	1:G:1733:TYR:N	2.41	0.53
3:I:1470:LEU:HD12	3:I:1489:ARG:HD2	1.90	0.53
1:B:1801:ASP:N	1:B:1801:ASP:OD1	2.40	0.53
2:D:1109:GLU:H	2:D:1188:GLN:HB2	1.74	0.53
1:F:1350:UNK:O	1:F:1357:UNK:N	2.42	0.53
1:G:451:ASN:O	1:G:469:ARG:NH1	2.41	0.53
2:A:689:GLY:O	2:A:693:LEU:N	2.39	0.53
2:E:1281:ASN:N	2:E:1281:ASN:OD1	2.38	0.53
1:F:1694:ALA:HA	1:F:1697:HIS:HB3	1.90	0.53
1:G:352:TYR:HA	1:G:355:LYS:HD2	1.89	0.53
1:G:368:ILE:HA	1:G:379:VAL:HG22	1.90	0.53
1:G:729:UNK:N	1:G:833:UNK:O	2.41	0.53
1:B:1740:THR:HB	1:B:1751:ILE:HD12	1.91	0.53
1:B:1716:ASN:O	1:B:1765:ARG:NE	2.41	0.53
2:D:1315:GLY:O	2:D:1318:THR:OG1	2.25	0.53
1:F:1716:ASN:O	1:F:1765:ARG:NE	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1714:PRO:HD2	1:B:1770:LEU:HB3	1.91	0.53
1:B:539:ASP:OD1	1:B:539:ASP:N	2.42	0.53
2:D:826:MET:N	2:D:867:ALA:O	2.38	0.53
1:F:156:LEU:O	1:F:268:LYS:N	2.40	0.53
1:F:361:PRO:HD2	1:F:364:LYS:HB2	1.90	0.53
2:A:374:UNK:O	2:A:378:UNK:N	2.42	0.53
1:B:352:TYR:HA	1:B:355:LYS:HD2	1.89	0.53
2:D:807:LYS:NZ	2:D:816:GLU:OE2	2.39	0.53
2:D:874:GLY:HA3	2:D:899:LYS:HD3	1.91	0.53
1:F:368:ILE:HA	1:F:379:VAL:HG22	1.90	0.53
1:G:122:LEU:HA	1:G:125:ASN:HB2	1.91	0.53
1:G:1350:UNK:O	1:G:1357:UNK:N	2.42	0.53
1:G:1390:UNK:O	1:G:1423:UNK:N	2.42	0.53
1:B:1679:ASP:OD2	1:B:1679:ASP:N	2.38	0.53
1:B:1729:ILE:O	1:B:1733:TYR:N	2.41	0.53
1:B:156:LEU:O	1:B:268:LYS:N	2.40	0.53
1:B:764:UNK:O	1:B:768:UNK:N	2.42	0.53
2:D:1110:LEU:HB3	2:D:1188:GLN:HA	1.90	0.53
2:D:1029:PRO:O	2:D:1193:TRP:NE1	2.41	0.53
2:E:1110:LEU:HB3	2:E:1188:GLN:HA	1.90	0.53
2:E:849:LEU:O	2:E:853:TRP:N	2.42	0.53
1:F:1283:UNK:O	1:F:1287:UNK:N	2.42	0.53
1:G:764:UNK:O	1:G:768:UNK:N	2.42	0.53
1:B:1314:UNK:N	1:B:1359:UNK:O	2.42	0.52
1:B:1390:UNK:O	1:B:1423:UNK:N	2.42	0.52
1:B:268:LYS:NZ	1:B:497:LYS:O	2.36	0.52
1:F:1790:GLU:O	1:F:1794:SER:N	2.41	0.52
1:G:1314:UNK:N	1:G:1359:UNK:O	2.42	0.52
1:G:1716:ASN:O	1:G:1765:ARG:NE	2.41	0.52
1:G:6:THR:O	1:G:7:ARG:NH1	2.37	0.52
2:E:824:LEU:O	2:E:867:ALA:N	2.39	0.52
1:G:1382:UNK:HA	1:G:1430:UNK:HA	1.91	0.52
1:B:1350:UNK:O	1:B:1357:UNK:N	2.42	0.52
1:B:368:ILE:HA	1:B:379:VAL:HG22	1.90	0.52
1:B:451:ASN:O	1:B:469:ARG:NH1	2.41	0.52
1:B:165:ASN:ND2	1:B:510:SER:O	2.42	0.52
2:E:1189:ILE:HD12	2:E:1378:GLU:HG3	1.92	0.52
1:G:159:ILE:O	1:G:504:PHE:N	2.39	0.52
1:G:1698:PHE:O	1:G:1702:TYR:N	2.37	0.52
1:B:1790:GLU:O	1:B:1794:SER:N	2.41	0.52
2:E:1327:CYS:SG	2:E:1328:ILE:N	2.78	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:UNK:O	2:E:378:UNK:N	2.42	0.52
1:F:1314:UNK:N	1:F:1359:UNK:O	2.42	0.52
1:F:1390:UNK:O	1:F:1423:UNK:N	2.42	0.52
2:A:935:GLU:OE2	2:A:938:GLU:N	2.32	0.52
1:B:1382:UNK:HA	1:B:1430:UNK:HA	1.91	0.52
2:D:374:UNK:O	2:D:378:UNK:N	2.42	0.52
2:E:1029:PRO:O	2:E:1193:TRP:NE1	2.41	0.52
1:G:361:PRO:HD2	1:G:364:LYS:HB2	1.91	0.52
1:G:165:ASN:ND2	1:G:510:SER:O	2.42	0.52
2:A:1327:CYS:SG	2:A:1328:ILE:N	2.77	0.52
2:D:1189:ILE:HD12	2:D:1378:GLU:HG3	1.92	0.52
2:D:744:ASP:N	2:D:744:ASP:OD1	2.37	0.52
2:E:1196:LYS:NZ	2:E:1198:TYR:OH	2.40	0.52
1:F:260:PRO:O	1:F:264:ARG:N	2.40	0.52
2:D:1327:CYS:SG	2:D:1328:ILE:N	2.78	0.52
1:F:1698:PHE:O	1:F:1702:TYR:N	2.37	0.52
1:F:1801:ASP:OD1	1:F:1801:ASP:N	2.40	0.52
1:F:25:ALA:O	1:F:29:ILE:N	2.43	0.52
1:F:764:UNK:O	1:F:768:UNK:N	2.43	0.52
1:G:1295:UNK:O	1:G:1299:UNK:N	2.43	0.52
2:A:849:LEU:O	2:A:853:TRP:N	2.42	0.52
2:D:1246:CYS:SG	2:D:1247:SER:N	2.82	0.52
1:G:539:ASP:OD1	1:G:539:ASP:N	2.42	0.52
2:A:874:GLY:HA3	2:A:899:LYS:HD3	1.91	0.52
2:E:1246:CYS:SG	2:E:1247:SER:N	2.82	0.52
1:G:705:UNK:O	1:G:709:UNK:N	2.43	0.52
1:B:1295:UNK:O	1:B:1299:UNK:N	2.43	0.52
1:B:974:UNK:O	1:B:978:UNK:N	2.43	0.52
1:F:384:GLN:O	1:F:388:GLY:N	2.43	0.52
1:F:165:ASN:ND2	1:F:510:SER:O	2.42	0.52
1:F:653:UNK:O	1:F:657:UNK:N	2.43	0.52
1:B:1283:UNK:O	1:B:1287:UNK:N	2.42	0.51
1:B:1769:GLY:O	1:B:1772:SER:OG	2.23	0.51
1:B:653:UNK:O	1:B:657:UNK:N	2.43	0.51
2:E:1055:TRP:HD1	2:E:1060:ILE:HD11	1.75	0.51
2:E:1131:LEU:HG	2:E:1133:PRO:HD3	1.92	0.51
2:E:1289:MET:HG3	2:E:1290:LEU:HD12	1.92	0.51
2:E:874:GLY:HA3	2:E:899:LYS:HD3	1.91	0.51
1:F:122:LEU:HA	1:F:125:ASN:HB2	1.91	0.51
1:G:1283:UNK:O	1:G:1287:UNK:N	2.42	0.51
2:A:1055:TRP:HD1	2:A:1060:ILE:HD11	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1131:LEU:HG	2:D:1133:PRO:HD3	1.92	0.51
1:F:1295:UNK:O	1:F:1299:UNK:N	2.43	0.51
1:F:1915:ASN:HB2	1:F:1917:ILE:HD11	1.92	0.51
1:F:345:THR:OG1	1:F:348:GLN:OE1	2.26	0.51
1:F:383:PRO:O	1:F:387:TYR:N	2.39	0.51
1:F:539:ASP:OD1	1:F:539:ASP:N	2.42	0.51
1:G:653:UNK:O	1:G:657:UNK:N	2.43	0.51
2:A:1015:LEU:HD12	2:A:1016:GLU:HB2	1.92	0.51
1:B:386:LEU:O	1:B:390:ASN:ND2	2.44	0.51
1:F:1713:ASN:OD1	1:F:1770:LEU:N	2.43	0.51
1:F:386:LEU:O	1:F:390:ASN:ND2	2.44	0.51
1:G:104:LEU:O	1:G:108:LEU:N	2.44	0.51
1:G:1714:PRO:HD2	1:G:1770:LEU:HB3	1.91	0.51
1:G:1915:ASN:HB2	1:G:1917:ILE:HD11	1.92	0.51
2:A:1196:LYS:NZ	2:A:1198:TYR:OH	2.40	0.51
2:A:1246:CYS:SG	2:A:1247:SER:N	2.82	0.51
1:B:1915:ASN:HB2	1:B:1917:ILE:HD11	1.92	0.51
1:B:25:ALA:O	1:B:29:ILE:N	2.43	0.51
2:D:689:GLY:O	2:D:693:LEU:N	2.39	0.51
1:G:113:ASP:OD1	1:G:113:ASP:N	2.44	0.51
1:G:1713:ASN:OD1	1:G:1770:LEU:N	2.43	0.51
1:F:705:UNK:O	1:F:709:UNK:N	2.43	0.51
1:F:974:UNK:O	1:F:978:UNK:N	2.43	0.51
1:G:974:UNK:O	1:G:978:UNK:N	2.43	0.51
2:A:722:TYR:HB2	2:A:732:LEU:HG	1.93	0.51
1:B:1681:TYR:O	1:B:1688:GLN:NE2	2.44	0.51
2:D:1055:TRP:HD1	2:D:1060:ILE:HD11	1.75	0.51
2:E:809:GLN:OE1	2:E:813:ARG:NH1	2.40	0.51
2:E:935:GLU:OE2	2:E:938:GLU:N	2.33	0.51
1:F:1335:UNK:O	1:F:1380:UNK:N	2.44	0.51
1:F:92:GLU:HA	1:F:96:LEU:HD21	1.93	0.51
1:G:1740:THR:HB	1:G:1751:ILE:HD12	1.91	0.51
2:A:809:GLN:OE1	2:A:813:ARG:NH1	2.40	0.51
2:E:787:LYS:O	2:E:791:ALA:N	2.43	0.51
1:F:1714:PRO:HD2	1:F:1770:LEU:HB3	1.91	0.51
1:F:318:SER:OG	1:G:1259:UNK:O	2.24	0.51
2:A:1046:SER:O	2:A:1049:GLY:N	2.31	0.51
2:A:1189:ILE:HD12	2:A:1378:GLU:HG3	1.92	0.51
1:B:1335:UNK:HA	1:B:1344:UNK:HA	1.93	0.51
2:D:1046:SER:O	2:D:1046:SER:OG	2.27	0.51
2:D:1289:MET:HG3	2:D:1290:LEU:HD12	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:722:TYR:HB2	2:D:732:LEU:HG	1.93	0.51
1:G:1:MET:H3	1:G:11:LEU:HD23	1.76	0.51
1:G:1681:TYR:O	1:G:1688:GLN:NE2	2.44	0.51
2:A:1131:LEU:HG	2:A:1133:PRO:HD3	1.92	0.51
1:B:705:UNK:O	1:B:709:UNK:N	2.43	0.51
1:F:104:LEU:O	1:F:108:LEU:N	2.44	0.51
1:F:1382:UNK:HA	1:F:1430:UNK:HA	1.91	0.51
2:A:1289:MET:HG3	2:A:1290:LEU:HD12	1.92	0.50
2:A:786:SER:O	2:A:788:SER:OG	2.27	0.50
2:A:807:LYS:NZ	2:A:816:GLU:OE2	2.39	0.50
2:A:887:GLY:HA2	2:A:890:LYS:HB2	1.93	0.50
1:B:6:THR:O	1:B:7:ARG:NH1	2.37	0.50
2:E:1175:ILE:HG12	2:E:1176:PRO:HA	1.93	0.50
2:E:687:SER:OG	2:E:688:ILE:N	2.43	0.50
1:G:1813:ALA:HA	1:G:1816:ALA:HB3	1.93	0.50
2:A:1120:GLU:HG2	2:A:1184:LEU:HD23	1.93	0.50
2:A:371:UNK:O	2:A:375:UNK:N	2.45	0.50
1:B:248:HIS:O	1:B:252:THR:OG1	2.25	0.50
1:B:92:GLU:HA	1:B:96:LEU:HD21	1.93	0.50
2:D:805:CYS:HA	2:D:808:LYS:HB2	1.93	0.50
2:E:661:ASP:O	2:E:665:LYS:N	2.44	0.50
2:E:805:CYS:HA	2:E:808:LYS:HB2	1.93	0.50
1:G:1335:UNK:HA	1:G:1344:UNK:HA	1.93	0.50
1:B:1713:ASN:OD1	1:B:1770:LEU:N	2.43	0.50
2:D:1015:LEU:HD12	2:D:1016:GLU:HB2	1.92	0.50
2:D:706:THR:HB	2:D:737:PHE:HB3	1.94	0.50
1:F:1312:UNK:N	1:F:1361:UNK:O	2.44	0.50
1:F:59:GLU:O	1:F:63:LYS:N	2.43	0.50
1:G:1335:UNK:O	1:G:1380:UNK:N	2.44	0.50
1:B:1335:UNK:O	1:B:1380:UNK:N	2.44	0.50
2:E:1703:UNK:O	2:E:1707:UNK:N	2.45	0.50
1:F:1681:TYR:O	1:F:1688:GLN:NE2	2.44	0.50
1:G:1637:LEU:HA	1:G:1657:ILE:HA	1.94	0.50
2:A:1086:ASP:N	2:A:1086:ASP:OD1	2.44	0.50
2:A:1703:UNK:O	2:A:1707:UNK:N	2.45	0.50
1:B:1312:UNK:N	1:B:1361:UNK:O	2.44	0.50
1:B:267:LEU:HD12	1:B:457:ILE:HG13	1.94	0.50
2:D:1120:GLU:HG2	2:D:1184:LEU:HD23	1.93	0.50
2:D:824:LEU:O	2:D:867:ALA:N	2.39	0.50
2:E:1120:GLU:HG2	2:E:1184:LEU:HD23	1.93	0.50
1:G:386:LEU:O	1:G:390:ASN:ND2	2.44	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:O	1:B:108:LEU:N	2.44	0.50
2:E:1015:LEU:HD12	2:E:1016:GLU:HB2	1.92	0.50
1:F:1698:PHE:HB3	1:F:1706:ILE:HD11	1.94	0.50
1:F:248:HIS:O	1:F:252:THR:OG1	2.25	0.50
1:G:1756:ASN:OD1	1:G:1759:SER:OG	2.29	0.50
2:D:1257:LEU:HD12	2:D:1260:MET:HB3	1.94	0.50
2:D:787:LYS:O	2:D:791:ALA:N	2.43	0.50
2:D:887:GLY:HA2	2:D:890:LYS:HB2	1.93	0.50
1:F:1756:ASN:OD1	1:F:1759:SER:OG	2.29	0.50
1:G:1312:UNK:N	1:G:1361:UNK:O	2.44	0.50
2:A:826:MET:N	2:A:867:ALA:O	2.38	0.50
1:B:59:GLU:O	1:B:63:LYS:N	2.43	0.50
3:C:1478:PRO:HB3	3:C:1482:GLN:HA	1.93	0.50
1:G:260:PRO:O	1:G:264:ARG:N	2.40	0.50
1:G:92:GLU:HA	1:G:96:LEU:HD21	1.93	0.50
1:G:94:CYS:SG	1:G:95:TYR:N	2.85	0.50
1:B:1813:ALA:HA	1:B:1816:ALA:HB3	1.93	0.50
2:D:1703:UNK:O	2:D:1707:UNK:N	2.45	0.50
1:F:1637:LEU:HA	1:F:1657:ILE:HA	1.94	0.50
1:F:259:THR:OG1	1:F:262:GLU:N	2.39	0.50
2:A:805:CYS:HA	2:A:808:LYS:HB2	1.93	0.49
1:B:371:VAL:HB	1:B:489:LYS:HA	1.94	0.49
2:E:371:UNK:O	2:E:375:UNK:N	2.45	0.49
1:F:1813:ALA:HA	1:F:1816:ALA:HB3	1.93	0.49
1:G:384:GLN:O	1:G:388:GLY:N	2.43	0.49
1:G:268:LYS:HZ3	1:G:497:LYS:HB2	1.77	0.49
2:A:1175:ILE:HG12	2:A:1176:PRO:HA	1.93	0.49
2:A:661:ASP:O	2:A:665:LYS:N	2.44	0.49
2:A:765:LEU:HD21	2:A:768:ILE:HD11	1.94	0.49
1:B:1674:GLN:OE1	1:B:1713:ASN:N	2.45	0.49
2:E:1046:SER:OG	2:E:1046:SER:O	2.27	0.49
2:E:887:GLY:HA2	2:E:890:LYS:HB2	1.93	0.49
1:F:765:UNK:O	1:F:769:UNK:N	2.45	0.49
1:B:1698:PHE:HB3	1:B:1706:ILE:HD11	1.94	0.49
1:B:186:ASP:N	1:B:186:ASP:OD1	2.45	0.49
1:F:113:ASP:N	1:F:113:ASP:OD1	2.44	0.49
1:F:1346:UNK:N	1:F:1362:UNK:O	2.46	0.49
1:G:1273:UNK:N	1:G:1321:UNK:O	2.46	0.49
2:E:1055:TRP:HA	2:E:1060:ILE:HG12	1.94	0.49
2:E:722:TYR:HB2	2:E:732:LEU:HG	1.93	0.49
2:E:755:THR:OG1	2:E:758:ASN:ND2	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1698:PHE:HB3	1:G:1706:ILE:HD11	1.94	0.49
3:I:1478:PRO:HB3	3:I:1482:GLN:HA	1.93	0.49
1:B:1346:UNK:N	1:B:1362:UNK:O	2.45	0.49
1:B:1637:LEU:HA	1:B:1657:ILE:HA	1.94	0.49
2:D:1248:GLY:HA2	2:D:1330:GLY:HA2	1.94	0.49
2:D:371:UNK:O	2:D:375:UNK:N	2.45	0.49
1:F:1878:VAL:HB	1:F:1898:TYR:HE1	1.77	0.49
1:G:765:UNK:O	1:G:769:UNK:N	2.45	0.49
3:H:1478:PRO:HB3	3:H:1482:GLN:HA	1.93	0.49
2:A:706:THR:HB	2:A:737:PHE:HB3	1.93	0.49
1:B:765:UNK:O	1:B:769:UNK:N	2.45	0.49
2:D:1175:ILE:HG12	2:D:1176:PRO:HA	1.93	0.49
2:D:755:THR:OG1	2:D:758:ASN:ND2	2.46	0.49
2:E:1096:SER:HA	2:E:1099:GLU:HB2	1.95	0.49
1:F:268:LYS:NZ	1:F:497:LYS:O	2.36	0.49
1:F:94:CYS:SG	1:F:95:TYR:N	2.85	0.49
1:G:1346:UNK:N	1:G:1362:UNK:O	2.46	0.49
1:G:1742:VAL:HG13	1:G:1751:ILE:HD11	1.94	0.49
2:A:755:THR:OG1	2:A:758:ASN:ND2	2.46	0.49
1:B:1:MET:H3	1:B:11:LEU:HD23	1.77	0.49
1:B:1259:UNK:O	1:G:318:SER:OG	2.27	0.49
1:G:186:ASP:N	1:G:186:ASP:OD1	2.45	0.49
2:A:840:SER:OG	2:A:841:GLU:N	2.46	0.49
1:B:1273:UNK:N	1:B:1321:UNK:O	2.46	0.49
2:D:687:SER:OG	2:D:688:ILE:N	2.43	0.49
2:E:706:THR:HB	2:E:737:PHE:HB3	1.93	0.49
2:A:1094:GLU:HA	2:A:1098:LEU:HD23	1.95	0.49
1:B:368:ILE:HD11	1:B:377:LEU:HD22	1.95	0.49
1:B:94:CYS:SG	1:B:95:TYR:N	2.85	0.49
2:D:661:ASP:O	2:D:665:LYS:N	2.44	0.49
2:E:765:LEU:HD21	2:E:768:ILE:HD11	1.94	0.49
1:F:1273:UNK:N	1:F:1321:UNK:O	2.46	0.49
2:A:1055:TRP:HA	2:A:1060:ILE:HG12	1.94	0.49
2:A:1113:GLY:HA2	2:A:1117:GLU:HA	1.95	0.49
2:A:1198:TYR:CZ	2:A:1217:VAL:HG21	2.48	0.49
1:B:1756:ASN:OD1	1:B:1759:SER:OG	2.29	0.49
2:E:1257:LEU:HD12	2:E:1260:MET:HB3	1.94	0.49
1:F:371:VAL:HB	1:F:489:LYS:HA	1.94	0.49
1:F:267:LEU:HD12	1:F:457:ILE:HG13	1.94	0.49
1:G:1878:VAL:HB	1:G:1898:TYR:HE1	1.77	0.49
1:G:267:LEU:HD12	1:G:457:ILE:HG13	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1257:LEU:HD12	2:A:1260:MET:HB3	1.94	0.48
2:A:787:LYS:O	2:A:791:ALA:N	2.43	0.48
1:B:260:PRO:HA	1:B:263:LEU:HB2	1.95	0.48
1:B:260:PRO:O	1:B:264:ARG:N	2.40	0.48
1:B:384:GLN:O	1:B:388:GLY:N	2.43	0.48
3:C:1457:ALA:O	3:C:1461:ASP:N	2.46	0.48
2:E:1319:ILE:HD11	2:E:1389:GLN:HG3	1.95	0.48
2:A:1248:GLY:HA2	2:A:1330:GLY:HA2	1.94	0.48
2:A:1436:VAL:O	2:A:1518:ARG:NH2	2.46	0.48
2:D:1055:TRP:HA	2:D:1060:ILE:HG12	1.94	0.48
2:D:1086:ASP:N	2:D:1086:ASP:OD1	2.44	0.48
2:D:1096:SER:HA	2:D:1099:GLU:HB2	1.95	0.48
2:D:1436:VAL:O	2:D:1518:ARG:NH2	2.46	0.48
2:E:1198:TYR:CZ	2:E:1217:VAL:HG21	2.48	0.48
1:F:1432:UNK:N	1:F:1440:UNK:O	2.46	0.48
1:F:2039:LYS:O	1:F:2043:ASP:N	2.45	0.48
1:G:1432:UNK:N	1:G:1440:UNK:O	2.46	0.48
1:G:368:ILE:HD11	1:G:377:LEU:HD22	1.95	0.48
2:A:1342:GLU:N	2:A:1345:ASN:OD1	2.47	0.48
2:A:778:GLY:N	2:A:835:GLY:O	2.46	0.48
1:B:253:ALA:O	1:B:258:PHE:N	2.37	0.48
2:D:754:ASP:HB3	2:D:758:ASN:HB2	1.95	0.48
2:D:765:LEU:HD21	2:D:768:ILE:HD11	1.94	0.48
2:D:857:SER:OG	2:D:857:SER:O	2.31	0.48
2:E:1436:VAL:O	2:E:1518:ARG:NH2	2.46	0.48
1:F:1105:UNK:O	1:F:1109:UNK:N	2.46	0.48
1:F:1335:UNK:HA	1:F:1344:UNK:HA	1.93	0.48
1:F:186:ASP:OD1	1:F:186:ASP:N	2.45	0.48
1:G:59:GLU:O	1:G:63:LYS:N	2.43	0.48
3:H:1502:ARG:O	3:H:1506:GLN:N	2.47	0.48
2:A:792:HIS:CD2	2:A:838:MET:HB3	2.49	0.48
1:B:2039:LYS:O	1:B:2043:ASP:N	2.45	0.48
1:B:84:LEU:O	1:B:88:LEU:N	2.45	0.48
2:D:1113:GLY:HA2	2:D:1117:GLU:HA	1.95	0.48
2:D:840:SER:OG	2:D:841:GLU:N	2.46	0.48
1:G:1105:UNK:O	1:G:1109:UNK:N	2.46	0.48
1:G:260:PRO:HA	1:G:263:LEU:HB2	1.95	0.48
1:G:371:VAL:HB	1:G:489:LYS:HA	1.94	0.48
3:I:1457:ALA:O	3:I:1461:ASP:N	2.46	0.48
2:A:687:SER:OG	2:A:688:ILE:N	2.43	0.48
2:A:824:LEU:H	2:A:866:GLY:HA2	1.79	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:OG1	1:B:348:GLN:OE1	2.26	0.48
2:D:1284:SER:O	2:D:1288:ASN:N	2.47	0.48
2:D:793:ARG:HG3	2:D:797:THR:HB	1.95	0.48
2:E:1248:GLY:HA2	2:E:1330:GLY:HA2	1.94	0.48
2:E:1342:GLU:N	2:E:1345:ASN:OD1	2.47	0.48
2:E:754:ASP:HB3	2:E:758:ASN:HB2	1.95	0.48
2:E:778:GLY:N	2:E:835:GLY:O	2.46	0.48
1:F:1674:GLN:OE1	1:F:1713:ASN:N	2.45	0.48
1:F:1758:HIS:CD2	1:F:1759:SER:H	2.32	0.48
2:A:1364:GLU:OE1	2:A:1367:ARG:NH2	2.45	0.48
2:E:1094:GLU:HA	2:E:1098:LEU:HD23	1.95	0.48
2:E:532:GLY:O	2:E:536:THR:N	2.46	0.48
1:F:1756:ASN:OD1	1:F:1756:ASN:N	2.47	0.48
1:G:1756:ASN:N	1:G:1756:ASN:OD1	2.47	0.48
1:B:1756:ASN:N	1:B:1756:ASN:OD1	2.47	0.48
2:D:1266:LYS:HD2	2:D:1266:LYS:HA	1.67	0.48
1:F:1849:ARG:HH22	1:F:1851:ASN:HA	1.78	0.48
1:G:1392:UNK:N	1:G:1421:UNK:O	2.46	0.48
1:G:2039:LYS:O	1:G:2043:ASP:N	2.45	0.48
1:G:525:VAL:HG22	1:G:554:GLY:H	1.79	0.48
2:A:1046:SER:OG	2:A:1046:SER:O	2.27	0.48
1:B:1105:UNK:O	1:B:1109:UNK:N	2.46	0.48
1:B:1392:UNK:N	1:B:1421:UNK:O	2.47	0.48
1:B:1878:VAL:HB	1:B:1898:TYR:HE1	1.77	0.48
1:B:194:THR:O	1:B:198:LEU:N	2.47	0.48
1:B:525:VAL:HG22	1:B:554:GLY:H	1.79	0.48
2:D:697:LEU:HD12	2:D:725:TYR:HB2	1.96	0.48
2:E:840:SER:OG	2:E:841:GLU:N	2.46	0.48
1:G:1758:HIS:CD2	1:G:1759:SER:H	2.32	0.48
2:A:1247:SER:HB3	2:A:1311:SER:HB2	1.96	0.48
2:A:697:LEU:HD12	2:A:725:TYR:HB2	1.96	0.48
1:B:1432:UNK:N	1:B:1440:UNK:O	2.46	0.48
3:C:1502:ARG:O	3:C:1506:GLN:N	2.47	0.48
2:D:1145:LYS:O	2:D:1149:GLY:N	2.41	0.48
2:D:1319:ILE:HD11	2:D:1389:GLN:HG3	1.95	0.48
2:D:711:SER:O	2:D:715:THR:OG1	2.28	0.48
2:E:1086:ASP:OD1	2:E:1086:ASP:N	2.44	0.48
2:E:1113:GLY:HA2	2:E:1117:GLU:HA	1.95	0.48
2:E:1160:THR:OG1	2:E:1166:LYS:NZ	2.44	0.48
1:F:1673:GLU:OE1	1:F:1675:GLY:N	2.47	0.48
2:A:1329:VAL:HG12	2:A:1385:GLN:H	1.79	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:O	1:B:130:ARG:N	2.47	0.48
1:B:1742:VAL:HG13	1:B:1751:ILE:HD11	1.95	0.48
1:B:1758:HIS:CD2	1:B:1759:SER:H	2.32	0.48
2:D:1198:TYR:CZ	2:D:1217:VAL:HG21	2.48	0.48
2:D:1342:GLU:N	2:D:1345:ASN:OD1	2.47	0.48
2:E:697:LEU:HD12	2:E:725:TYR:HB2	1.96	0.48
2:E:824:LEU:H	2:E:866:GLY:HA2	1.79	0.48
1:F:525:VAL:HG22	1:F:554:GLY:H	1.79	0.48
1:G:25:ALA:O	1:G:29:ILE:N	2.43	0.48
2:A:711:SER:O	2:A:715:THR:OG1	2.28	0.47
1:B:1750:LYS:O	1:B:1753:LYS:NZ	2.35	0.47
2:D:1352:THR:OG1	2:D:1353:LEU:N	2.47	0.47
2:D:824:LEU:H	2:D:866:GLY:HA2	1.79	0.47
1:F:368:ILE:HD11	1:F:377:LEU:HD22	1.95	0.47
1:F:435:ALA:HA	1:F:438:LEU:HB3	1.96	0.47
2:A:1352:THR:OG1	2:A:1353:LEU:N	2.47	0.47
1:B:1673:GLU:OE1	1:B:1675:GLY:N	2.47	0.47
1:B:1849:ARG:HH22	1:B:1851:ASN:HA	1.78	0.47
2:D:792:HIS:CD2	2:D:838:MET:HB3	2.49	0.47
2:D:809:GLN:OE1	2:D:813:ARG:NH1	2.40	0.47
2:E:1128:GLU:HB3	2:E:1177:LYS:HG2	1.97	0.47
1:F:1392:UNK:N	1:F:1421:UNK:O	2.47	0.47
1:F:194:THR:O	1:F:198:LEU:N	2.47	0.47
1:F:319:LEU:HD21	1:F:323:ILE:HB	1.96	0.47
1:G:1277:UNK:O	1:G:1279:UNK:N	2.47	0.47
1:G:63:LYS:NZ	1:G:63:LYS:O	2.38	0.47
3:H:1457:ALA:O	3:H:1461:ASP:N	2.46	0.47
3:H:1506:GLN:O	3:H:1511:ASP:N	2.47	0.47
3:I:1502:ARG:O	3:I:1506:GLN:N	2.47	0.47
2:E:1514:LYS:N	3:I:1513:TYR:O	2.48	0.47
2:A:1319:ILE:HD11	2:A:1389:GLN:HG3	1.95	0.47
1:F:170:PHE:O	1:F:174:ARG:N	2.40	0.47
2:D:1514:LYS:N	3:H:1513:TYR:O	2.48	0.47
1:B:1277:UNK:O	1:B:1279:UNK:N	2.47	0.47
2:D:778:GLY:N	2:D:835:GLY:O	2.46	0.47
1:F:1721:PHE:O	1:F:1733:TYR:OH	2.25	0.47
2:A:792:HIS:CD2	2:A:842:SER:HB3	2.49	0.47
2:E:1207:GLN:NE2	2:E:1277:GLU:OE1	2.40	0.47
2:E:792:HIS:CD2	2:E:838:MET:HB3	2.49	0.47
1:F:1742:VAL:HG13	1:F:1751:ILE:HD11	1.94	0.47
2:A:1096:SER:HA	2:A:1099:GLU:HB2	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1514:LYS:N	3:C:1513:TYR:O	2.48	0.47
2:A:1729:UNK:O	2:A:1733:UNK:N	2.48	0.47
2:D:1094:GLU:HA	2:D:1098:LEU:HD23	1.95	0.47
2:E:798:ASN:N	2:E:798:ASN:OD1	2.48	0.47
1:G:1674:GLN:OE1	1:G:1713:ASN:N	2.45	0.47
1:G:1741:ILE:HD11	1:G:1748:THR:HA	1.97	0.47
1:G:383:PRO:O	1:G:387:TYR:N	2.39	0.47
3:I:1506:GLN:O	3:I:1511:ASP:N	2.47	0.47
2:A:1145:LYS:O	2:A:1149:GLY:N	2.41	0.47
2:A:1284:SER:O	2:A:1288:ASN:N	2.47	0.47
2:A:754:ASP:HB3	2:A:758:ASN:HB2	1.96	0.47
3:C:1506:GLN:O	3:C:1511:ASP:N	2.47	0.47
2:D:1247:SER:HB3	2:D:1311:SER:HB2	1.96	0.47
2:D:1329:VAL:HG12	2:D:1385:GLN:H	1.79	0.47
2:E:1275:LEU:O	2:E:1278:SER:OG	2.30	0.47
2:E:792:HIS:CD2	2:E:842:SER:HB3	2.49	0.47
1:F:1741:ILE:HD11	1:F:1748:THR:HA	1.97	0.47
1:G:108:LEU:HB3	1:G:119:THR:HG23	1.96	0.47
2:A:1266:LYS:HD2	2:A:1266:LYS:HA	1.67	0.47
2:A:532:GLY:O	2:A:536:THR:N	2.46	0.47
2:A:753:TYR:OH	2:A:764:ASP:O	2.24	0.47
2:A:780:GLU:HG2	2:A:781:LEU:HG	1.97	0.47
1:B:170:PHE:O	1:B:174:ARG:N	2.40	0.47
1:B:319:LEU:HD21	1:B:323:ILE:HB	1.96	0.47
2:D:1160:THR:OG1	2:D:1166:LYS:NZ	2.44	0.47
2:E:1247:SER:HB3	2:E:1311:SER:HB2	1.96	0.47
2:E:1312:VAL:O	2:E:1316:VAL:N	2.42	0.47
2:E:1352:THR:OG1	2:E:1353:LEU:N	2.47	0.47
2:E:826:MET:N	2:E:867:ALA:O	2.38	0.47
1:F:63:LYS:HA	1:F:63:LYS:HD2	1.77	0.47
2:A:793:ARG:HG3	2:A:797:THR:HB	1.95	0.47
2:E:793:ARG:HG3	2:E:797:THR:HB	1.95	0.47
1:F:1277:UNK:O	1:F:1279:UNK:N	2.47	0.47
1:F:184:VAL:HG22	1:F:188:ILE:HG12	1.97	0.47
1:F:1:MET:H3	1:F:11:LEU:HD23	1.79	0.47
2:A:857:SER:OG	2:A:857:SER:O	2.31	0.47
2:E:1329:VAL:HG12	2:E:1385:GLN:H	1.79	0.47
1:F:108:LEU:HB3	1:F:119:THR:HG23	1.96	0.47
1:G:170:PHE:O	1:G:174:ARG:N	2.40	0.47
1:G:1849:ARG:HH22	1:G:1851:ASN:HA	1.78	0.47
1:B:268:LYS:HZ3	1:B:497:LYS:HB2	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:780:GLU:HG2	2:D:781:LEU:HG	1.97	0.47
2:D:792:HIS:CD2	2:D:842:SER:HB3	2.49	0.47
2:E:1284:SER:O	2:E:1288:ASN:N	2.47	0.47
1:F:126:TYR:O	1:F:130:ARG:N	2.47	0.47
1:G:1213:UNK:O	1:G:1215:UNK:N	2.48	0.47
1:G:271:THR:O	1:G:271:THR:OG1	2.33	0.47
1:G:432:LEU:HD23	1:G:432:LEU:HA	1.73	0.47
1:B:171:GLU:OE2	1:B:174:ARG:NH2	2.48	0.46
2:D:1275:LEU:O	2:D:1278:SER:OG	2.30	0.46
1:F:157:VAL:O	1:F:502:LEU:N	2.48	0.46
1:G:1842:VAL:HG12	1:G:1844:ARG:HB2	1.97	0.46
2:A:1128:GLU:HB3	2:A:1177:LYS:HG2	1.97	0.46
1:B:1213:UNK:O	1:B:1215:UNK:N	2.48	0.46
1:B:435:ALA:HA	1:B:438:LEU:HB3	1.96	0.46
2:E:1145:LYS:O	2:E:1149:GLY:N	2.41	0.46
1:F:432:LEU:HA	1:F:432:LEU:HD23	1.73	0.46
1:G:194:THR:O	1:G:198:LEU:N	2.47	0.46
1:G:84:LEU:O	1:G:88:LEU:N	2.45	0.46
1:B:108:LEU:HB3	1:B:119:THR:HG23	1.96	0.46
1:B:238:CYS:HA	1:B:275:GLN:NE2	2.30	0.46
1:F:171:GLU:OE2	1:F:174:ARG:NH2	2.48	0.46
1:F:260:PRO:HA	1:F:263:LEU:HB2	1.96	0.46
1:F:238:CYS:HA	1:F:275:GLN:NE2	2.30	0.46
1:F:469:ARG:HD2	1:F:469:ARG:HA	1.57	0.46
1:G:162:GLY:HA3	1:G:275:GLN:HB3	1.98	0.46
2:A:1207:GLN:HA	2:A:1271:GLN:HE22	1.80	0.46
1:B:1665:VAL:HA	1:B:1805:ALA:HB3	1.98	0.46
1:B:1842:VAL:HG12	1:B:1844:ARG:HB2	1.97	0.46
2:D:1128:GLU:HB3	2:D:1177:LYS:HG2	1.97	0.46
1:F:1842:VAL:HG12	1:F:1844:ARG:HB2	1.97	0.46
1:F:271:THR:O	1:F:271:THR:OG1	2.33	0.46
1:G:171:GLU:OE2	1:G:174:ARG:NH2	2.48	0.46
1:B:1970:VAL:O	1:B:1974:VAL:N	2.49	0.46
1:B:63:LYS:HD2	1:B:63:LYS:HA	1.77	0.46
2:E:780:GLU:HG2	2:E:781:LEU:HG	1.97	0.46
1:F:1213:UNK:O	1:F:1215:UNK:N	2.48	0.46
1:G:1104:UNK:O	1:G:1106:UNK:N	2.49	0.46
1:B:157:VAL:O	1:B:502:LEU:N	2.48	0.46
2:D:1729:UNK:O	2:D:1733:UNK:N	2.48	0.46
1:F:1329:UNK:N	1:F:1349:UNK:O	2.49	0.46
1:F:1970:VAL:O	1:F:1974:VAL:N	2.49	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1329:UNK:N	1:G:1349:UNK:O	2.49	0.46
2:A:1168:LEU:HB3	2:A:1169:LYS:H	1.51	0.46
2:A:709:ARG:CZ	2:A:710:PHE:H	2.28	0.46
1:B:471:LEU:HG	1:B:472:SER:H	1.81	0.46
2:E:1729:UNK:O	2:E:1733:UNK:N	2.48	0.46
2:E:709:ARG:CZ	2:E:710:PHE:H	2.28	0.46
2:E:857:SER:OG	2:E:857:SER:O	2.30	0.46
1:F:162:GLY:HA3	1:F:275:GLN:HB3	1.98	0.46
1:G:184:VAL:HG22	1:G:188:ILE:HG12	1.97	0.46
1:B:63:LYS:O	1:B:63:LYS:NZ	2.38	0.46
2:D:532:GLY:O	2:D:536:THR:N	2.46	0.46
2:D:935:GLU:OE2	2:D:938:GLU:N	2.33	0.46
2:E:1207:GLN:HA	2:E:1271:GLN:HE22	1.80	0.46
2:E:1326:ILE:HG23	2:E:1388:MET:HG2	1.98	0.46
1:G:1768:LYS:HE2	1:G:1768:LYS:HB3	1.70	0.46
1:G:238:CYS:HA	1:G:275:GLN:NE2	2.30	0.46
1:G:253:ALA:O	1:G:258:PHE:N	2.37	0.46
1:G:766:UNK:O	1:G:771:UNK:N	2.49	0.46
1:B:160:PHE:H	1:B:272:GLY:HA2	1.81	0.46
1:B:1741:ILE:HD11	1:B:1748:THR:HA	1.97	0.46
1:B:403:ASP:OD1	1:B:403:ASP:N	2.49	0.46
1:F:471:LEU:HG	1:F:472:SER:H	1.81	0.46
1:F:84:LEU:O	1:F:88:LEU:N	2.45	0.46
1:G:126:TYR:O	1:G:130:ARG:N	2.47	0.46
1:G:435:ALA:HA	1:G:438:LEU:HB3	1.96	0.46
2:A:1326:ILE:HG23	2:A:1388:MET:HG2	1.98	0.46
1:B:1104:UNK:O	1:B:1106:UNK:N	2.49	0.46
1:B:1329:UNK:N	1:B:1349:UNK:O	2.49	0.46
1:B:162:GLY:HA3	1:B:275:GLN:HB3	1.98	0.46
1:F:1104:UNK:O	1:F:1106:UNK:N	2.49	0.46
1:F:766:UNK:O	1:F:771:UNK:N	2.49	0.46
1:G:1438:UNK:HA	1:G:1469:UNK:HA	1.97	0.46
1:G:364:LYS:HA	1:G:382:PRO:HG3	1.98	0.46
3:I:1448:ARG:HA	3:I:1451:GLN:HB3	1.97	0.46
1:B:3:ALA:N	1:B:9:LEU:O	2.39	0.45
3:C:1448:ARG:HA	3:C:1451:GLN:HB3	1.97	0.45
2:D:786:SER:O	2:D:788:SER:OG	2.27	0.45
2:D:902:ALA:HA	2:D:905:LEU:HD13	1.99	0.45
1:F:3:ALA:N	1:F:9:LEU:O	2.39	0.45
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.57	0.45
2:D:1516:ASP:OD2	2:D:1519:ILE:N	2.38	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1073:THR:OG1	2:E:1074:GLY:N	2.49	0.45
1:G:319:LEU:HD21	1:G:323:ILE:HB	1.96	0.45
1:G:326:ASP:HA	1:G:329:GLU:HG2	1.99	0.45
2:A:914:VAL:O	2:A:918:GLN:N	2.50	0.45
1:B:1923:ASP:HB3	1:B:1924:ILE:H	1.35	0.45
2:D:1168:LEU:HB3	2:D:1169:LYS:H	1.51	0.45
2:D:1326:ILE:HG23	2:D:1388:MET:HG2	1.98	0.45
2:D:709:ARG:CZ	2:D:710:PHE:H	2.28	0.45
2:D:710:PHE:HB2	2:D:736:PRO:HB3	1.99	0.45
2:E:1192:GLY:HA3	2:E:1193:TRP:CD2	2.52	0.45
1:G:1673:GLU:OE1	1:G:1675:GLY:N	2.47	0.45
1:G:229:ASP:HA	1:G:232:LEU:HD12	1.99	0.45
2:A:1162:GLU:HG2	2:A:1163:TYR:HD1	1.82	0.45
1:B:95:TYR:OH	1:B:111:GLU:OE1	2.35	0.45
1:B:1438:UNK:HA	1:B:1469:UNK:HA	1.97	0.45
1:B:29:ILE:HA	1:B:29:ILE:HD12	1.87	0.45
1:B:503:ASP:N	1:B:527:VAL:O	2.48	0.45
2:D:914:VAL:O	2:D:918:GLN:N	2.50	0.45
2:E:753:TYR:OH	2:E:764:ASP:O	2.24	0.45
1:F:469:ARG:HH12	1:F:471:LEU:HD13	1.81	0.45
1:G:345:THR:OG1	1:G:348:GLN:OE1	2.26	0.45
1:G:476:SER:OG	1:G:476:SER:O	2.33	0.45
2:A:902:ALA:HA	2:A:905:LEU:HD13	1.99	0.45
1:B:1147:UNK:N	1:B:1158:UNK:O	2.50	0.45
1:B:229:ASP:HA	1:B:232:LEU:HD12	1.98	0.45
1:B:383:PRO:O	1:B:387:TYR:N	2.39	0.45
2:E:1212:THR:HG22	2:E:1283:MET:HG3	1.99	0.45
1:F:1438:UNK:HA	1:F:1469:UNK:HA	1.97	0.45
1:F:160:PHE:H	1:F:272:GLY:HA2	1.81	0.45
1:F:1674:GLN:NE2	1:F:1710:VAL:O	2.50	0.45
1:F:229:ASP:HA	1:F:232:LEU:HD12	1.99	0.45
1:F:157:VAL:HB	1:F:501:ILE:HG12	1.99	0.45
1:G:1970:VAL:O	1:G:1974:VAL:N	2.49	0.45
1:G:469:ARG:HH12	1:G:471:LEU:HD13	1.81	0.45
3:H:1448:ARG:HA	3:H:1451:GLN:HB3	1.97	0.45
2:A:1281:ASN:OD1	2:A:1281:ASN:N	2.38	0.45
1:B:26:SER:HA	1:B:29:ILE:HG22	1.99	0.45
2:D:1259:GLY:HA2	2:D:1263:ASP:HB2	1.99	0.45
2:E:868:ILE:HG22	2:E:926:LEU:HD12	1.99	0.45
2:E:902:ALA:HA	2:E:905:LEU:HD13	1.99	0.45
1:F:403:ASP:N	1:F:403:ASP:OD1	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:821:GLN:HA	2:A:863:THR:HB	1.98	0.45
1:B:766:UNK:O	1:B:771:UNK:N	2.49	0.45
2:D:821:GLN:HA	2:D:863:THR:HB	1.98	0.45
1:F:1147:UNK:N	1:F:1158:UNK:O	2.50	0.45
1:F:1877:ARG:HA	1:F:1877:ARG:HD2	1.72	0.45
1:F:268:LYS:HZ3	1:F:497:LYS:HB2	1.81	0.45
1:G:1147:UNK:N	1:G:1158:UNK:O	2.50	0.45
1:G:26:SER:HA	1:G:29:ILE:HG22	1.99	0.45
1:G:309:ARG:O	1:G:313:ALA:N	2.48	0.45
2:A:1131:LEU:HD12	2:A:1132:GLU:H	1.81	0.45
2:A:1281:ASN:O	2:A:1284:SER:OG	2.33	0.45
1:B:364:LYS:HA	1:B:382:PRO:HG3	1.98	0.45
1:B:485:ARG:HA	1:B:485:ARG:HD2	1.82	0.45
2:D:1192:GLY:HA3	2:D:1193:TRP:CD2	2.52	0.45
2:E:1162:GLU:HG2	2:E:1163:TYR:HD1	1.82	0.45
1:F:1428:UNK:O	1:F:1444:UNK:N	2.50	0.45
1:G:1291:UNK:O	1:G:1295:UNK:N	2.50	0.45
2:A:847:GLU:N	2:A:847:GLU:OE1	2.50	0.45
1:B:433:VAL:O	1:B:436:SER:OG	2.27	0.45
2:E:821:GLN:HA	2:E:863:THR:HB	1.98	0.45
1:G:1396:UNK:O	1:G:1400:UNK:N	2.50	0.45
1:B:184:VAL:HG22	1:B:188:ILE:HG12	1.97	0.45
1:B:279:THR:O	1:B:283:ILE:N	2.49	0.45
1:B:326:ASP:HA	1:B:329:GLU:HG2	1.99	0.45
1:B:157:VAL:HB	1:B:501:ILE:HG12	1.98	0.45
1:B:741:UNK:O	1:B:745:UNK:N	2.50	0.45
1:F:1396:UNK:O	1:F:1400:UNK:N	2.50	0.45
1:F:159:ILE:O	1:F:504:PHE:N	2.39	0.45
1:F:85:ASN:HA	1:F:88:LEU:HD12	1.98	0.45
1:G:1728:ARG:HD3	1:G:1728:ARG:HA	1.74	0.45
1:B:469:ARG:HH12	1:B:471:LEU:HD13	1.81	0.44
2:D:1131:LEU:HD12	2:D:1132:GLU:H	1.81	0.44
2:D:1207:GLN:HA	2:D:1271:GLN:HE22	1.80	0.44
2:D:847:GLU:OE1	2:D:847:GLU:N	2.50	0.44
1:F:1291:UNK:O	1:F:1295:UNK:N	2.50	0.44
1:F:1923:ASP:HB3	1:F:1924:ILE:H	1.35	0.44
1:G:1428:UNK:O	1:G:1444:UNK:N	2.50	0.44
1:G:157:VAL:O	1:G:502:LEU:N	2.48	0.44
1:G:160:PHE:H	1:G:272:GLY:HA2	1.81	0.44
1:G:1674:GLN:NE2	1:G:1710:VAL:O	2.50	0.44
1:G:372:ASN:N	1:G:372:ASN:OD1	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:471:LEU:HG	1:G:472:SER:H	1.81	0.44
1:G:157:VAL:HB	1:G:501:ILE:HG12	1.98	0.44
2:A:1212:THR:HG22	2:A:1283:MET:HG3	1.99	0.44
2:A:1291:LEU:HA	2:A:1291:LEU:HD23	1.79	0.44
2:A:950:THR:HA	2:A:953:VAL:HG12	1.99	0.44
1:B:1428:UNK:O	1:B:1444:UNK:N	2.50	0.44
1:B:917:UNK:O	1:B:921:UNK:N	2.50	0.44
2:D:1056:ILE:HG23	2:D:1057:MET:HG3	2.00	0.44
2:D:739:GLN:NE2	2:D:794:ILE:O	2.51	0.44
1:F:253:ALA:O	1:F:258:PHE:N	2.37	0.44
1:F:917:UNK:O	1:F:921:UNK:N	2.50	0.44
1:G:95:TYR:OH	1:G:111:GLU:OE1	2.35	0.44
1:G:1745:LYS:HD3	1:G:1745:LYS:HA	1.80	0.44
1:G:85:ASN:HA	1:G:88:LEU:HD12	1.98	0.44
2:A:1073:THR:OG1	2:A:1074:GLY:N	2.49	0.44
2:A:798:ASN:OD1	2:A:798:ASN:N	2.48	0.44
1:B:1674:GLN:NE2	1:B:1710:VAL:O	2.50	0.44
1:B:1877:ARG:HA	1:B:1877:ARG:HD2	1.72	0.44
1:B:199:ILE:HG13	1:B:200:ARG:HD2	1.99	0.44
1:F:326:ASP:HA	1:F:329:GLU:HG2	1.99	0.44
1:F:340:SER:HB3	1:F:421:LEU:HD11	2.00	0.44
1:G:1673:GLU:OE2	1:G:1676:MET:N	2.43	0.44
2:A:1056:ILE:HG23	2:A:1057:MET:HG3	2.00	0.44
2:A:1275:LEU:O	2:A:1278:SER:OG	2.30	0.44
1:B:1291:UNK:O	1:B:1295:UNK:N	2.50	0.44
1:B:85:ASN:HA	1:B:88:LEU:HD12	1.98	0.44
1:F:1424:UNK:N	1:F:1448:UNK:O	2.51	0.44
1:G:1424:UNK:N	1:G:1448:UNK:O	2.51	0.44
2:A:1192:GLY:HA3	2:A:1193:TRP:CD2	2.52	0.44
1:B:116:LEU:O	1:B:120:LYS:N	2.46	0.44
1:B:175:ASP:HA	1:B:178:GLN:HE21	1.83	0.44
1:B:262:GLU:OE2	1:B:266:TYR:OH	2.24	0.44
1:B:372:ASN:OD1	1:B:372:ASN:N	2.48	0.44
2:D:1162:GLU:HG2	2:D:1163:TYR:HD1	1.82	0.44
2:E:1131:LEU:HD12	2:E:1132:GLU:H	1.81	0.44
2:E:1274:ILE:HA	2:E:1274:ILE:HD12	1.88	0.44
2:E:795:MET:N	2:E:795:MET:SD	2.91	0.44
1:G:246:LEU:HD11	1:G:296:VAL:HG22	2.00	0.44
2:A:1126:ILE:HG23	2:A:1179:LEU:HA	2.00	0.44
2:A:1418:VAL:HA	2:A:1419:PRO:HA	1.79	0.44
2:A:868:ILE:HG22	2:A:926:LEU:HD12	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1424:UNK:N	1:B:1448:UNK:O	2.51	0.44
2:D:798:ASN:OD1	2:D:798:ASN:N	2.48	0.44
2:D:875:THR:HG23	2:D:879:SER:HB3	2.00	0.44
2:E:1148:HIS:NE2	2:E:1153:ASP:OD2	2.47	0.44
2:E:710:PHE:HB2	2:E:736:PRO:HB3	1.99	0.44
2:E:950:THR:HA	2:E:953:VAL:HG12	1.99	0.44
1:F:1665:VAL:HA	1:F:1805:ALA:HB3	1.98	0.44
1:F:246:LEU:HD11	1:F:296:VAL:HG22	2.00	0.44
1:G:1308:UNK:HA	1:G:1364:UNK:HA	2.00	0.44
1:G:741:UNK:O	1:G:745:UNK:N	2.50	0.44
1:B:1308:UNK:HA	1:B:1364:UNK:HA	2.00	0.44
1:B:1396:UNK:O	1:B:1400:UNK:N	2.50	0.44
1:B:246:LEU:HD11	1:B:296:VAL:HG22	2.00	0.44
2:D:1353:LEU:HA	2:D:1356:PHE:HB3	2.00	0.44
2:D:868:ILE:HG22	2:D:926:LEU:HD12	1.99	0.44
2:E:875:THR:HG23	2:E:879:SER:HB3	2.00	0.44
2:E:914:VAL:O	2:E:918:GLN:N	2.50	0.44
1:F:1768:LYS:HE2	1:F:1768:LYS:HB3	1.69	0.44
1:F:364:LYS:HA	1:F:382:PRO:HG3	1.98	0.44
1:G:203:LEU:HA	1:G:203:LEU:HD13	1.89	0.44
2:A:1274:ILE:HA	2:A:1274:ILE:HD12	1.88	0.44
2:A:1326:ILE:HD12	2:A:1388:MET:HG2	2.00	0.44
1:B:113:ASP:OD1	1:B:113:ASP:N	2.44	0.44
1:B:1376:UNK:O	1:B:1378:UNK:N	2.51	0.44
2:E:711:SER:O	2:E:715:THR:OG1	2.28	0.44
1:F:1376:UNK:O	1:F:1378:UNK:N	2.51	0.44
1:F:477:GLU:O	1:F:481:ASP:N	2.48	0.44
1:G:310:CYS:O	1:G:314:TYR:N	2.40	0.44
1:G:682:UNK:O	1:G:686:UNK:N	2.51	0.44
1:G:917:UNK:O	1:G:921:UNK:N	2.50	0.44
2:A:710:PHE:HB2	2:A:736:PRO:HB3	1.99	0.44
2:A:739:GLN:NE2	2:A:794:ILE:O	2.51	0.44
2:A:826:MET:HG3	2:A:867:ALA:H	1.83	0.44
1:B:1768:LYS:HE2	1:B:1768:LYS:HB3	1.69	0.44
1:B:1863:ALA:HA	1:B:1866:PHE:HB3	2.00	0.44
1:B:926:UNK:O	1:B:930:UNK:N	2.50	0.44
2:E:1056:ILE:HG23	2:E:1057:MET:HG3	1.99	0.44
2:E:847:GLU:N	2:E:847:GLU:OE1	2.50	0.44
2:E:820:ALA:N	2:E:861:GLN:O	2.51	0.44
1:F:178:GLN:O	1:F:181:HIS:NE2	2.51	0.44
1:F:38:ASN:HA	1:F:41:LEU:HG	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:682:UNK:O	1:F:686:UNK:N	2.51	0.44
3:I:1456:GLU:H	3:I:1459:ILE:HG12	1.83	0.44
1:B:1673:GLU:OE2	1:B:1676:MET:N	2.43	0.43
1:B:1715:VAL:O	1:B:1717:LEU:N	2.51	0.43
2:D:1126:ILE:HG23	2:D:1179:LEU:HA	2.00	0.43
2:D:826:MET:HG3	2:D:867:ALA:H	1.83	0.43
2:E:1259:GLY:HA2	2:E:1263:ASP:HB2	1.99	0.43
2:E:1353:LEU:HA	2:E:1356:PHE:HB3	2.00	0.43
2:E:826:MET:HG3	2:E:867:ALA:H	1.83	0.43
1:F:1308:UNK:HA	1:F:1364:UNK:HA	2.00	0.43
1:F:175:ASP:HA	1:F:178:GLN:HE21	1.83	0.43
1:F:199:ILE:HG13	1:F:200:ARG:HD2	1.99	0.43
1:F:926:UNK:O	1:F:930:UNK:N	2.50	0.43
1:G:175:ASP:HA	1:G:178:GLN:HE21	1.83	0.43
1:G:199:ILE:HG13	1:G:200:ARG:HD2	1.99	0.43
1:G:285:GLU:HG3	1:G:298:LYS:HZ3	1.83	0.43
2:A:820:ALA:O	2:A:863:THR:N	2.51	0.43
1:B:1728:ARG:HD3	1:B:1728:ARG:HA	1.74	0.43
1:B:682:UNK:O	1:B:686:UNK:N	2.51	0.43
2:D:1212:THR:HG22	2:D:1283:MET:HG3	1.99	0.43
2:E:1168:LEU:HB3	2:E:1169:LYS:H	1.51	0.43
1:F:26:SER:HA	1:F:29:ILE:HG22	1.99	0.43
1:F:741:UNK:O	1:F:745:UNK:N	2.50	0.43
1:G:1376:UNK:O	1:G:1378:UNK:N	2.51	0.43
1:G:1923:ASP:HB3	1:G:1924:ILE:H	1.36	0.43
1:G:404:GLN:HA	1:G:408:PRO:HB3	2.00	0.43
1:G:340:SER:HB3	1:G:421:LEU:HD11	2.00	0.43
1:B:340:SER:HB3	1:B:421:LEU:HD11	2.00	0.43
2:E:1281:ASN:O	2:E:1284:SER:OG	2.33	0.43
1:F:1718:THR:HG21	1:F:1770:LEU:HD13	2.00	0.43
1:F:482:CYS:HA	1:F:486:LEU:HD12	2.01	0.43
1:G:1665:VAL:HA	1:G:1805:ALA:HB3	1.98	0.43
1:G:1718:THR:HG21	1:G:1770:LEU:HD13	2.00	0.43
1:G:403:ASP:OD1	1:G:403:ASP:N	2.49	0.43
1:G:926:UNK:O	1:G:930:UNK:N	2.51	0.43
3:H:1456:GLU:H	3:H:1459:ILE:HG12	1.83	0.43
2:A:1160:THR:OG1	2:A:1166:LYS:NZ	2.44	0.43
2:A:1394:LEU:HA	2:A:1394:LEU:HD23	1.84	0.43
2:D:732:LEU:HD13	2:D:732:LEU:HA	1.82	0.43
1:F:1214:UNK:O	1:F:1218:UNK:N	2.52	0.43
1:F:1715:VAL:O	1:F:1717:LEU:N	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:503:ASP:N	1:F:527:VAL:O	2.48	0.43
2:A:1259:GLY:HA2	2:A:1263:ASP:HB2	1.99	0.43
1:B:178:GLN:O	1:B:181:HIS:NE2	2.51	0.43
2:D:1326:ILE:HD12	2:D:1388:MET:HG2	2.00	0.43
1:F:1765:ARG:NH2	1:F:1767:GLU:OE2	2.52	0.43
1:F:309:ARG:O	1:F:313:ALA:N	2.48	0.43
1:G:1214:UNK:O	1:G:1218:UNK:N	2.52	0.43
1:G:417:SER:O	1:G:417:SER:OG	2.37	0.43
1:B:390:ASN:HA	1:B:393:LEU:HB2	2.00	0.43
3:C:1456:GLU:H	3:C:1459:ILE:HG12	1.83	0.43
2:D:1312:VAL:O	2:D:1316:VAL:N	2.42	0.43
2:D:403:UNK:O	2:D:407:UNK:N	2.51	0.43
2:D:925:ASP:N	2:D:925:ASP:OD1	2.34	0.43
1:F:1472:UNK:O	1:F:1476:UNK:N	2.52	0.43
1:F:1728:ARG:HA	1:F:1728:ARG:HD3	1.74	0.43
1:G:29:ILE:HD12	1:G:29:ILE:HA	1.87	0.43
1:B:159:ILE:O	1:B:504:PHE:N	2.39	0.43
1:B:482:CYS:HA	1:B:486:LEU:HD12	2.01	0.43
2:D:1073:THR:OG1	2:D:1074:GLY:N	2.49	0.43
2:D:1418:VAL:HA	2:D:1419:PRO:HA	1.79	0.43
2:D:795:MET:SD	2:D:795:MET:N	2.91	0.43
2:D:950:THR:HA	2:D:953:VAL:HG12	1.99	0.43
1:F:390:ASN:HA	1:F:393:LEU:HB2	2.00	0.43
1:F:417:SER:OG	1:F:417:SER:O	2.37	0.43
1:F:156:LEU:HD21	1:F:502:LEU:HD12	2.01	0.43
1:G:1715:VAL:O	1:G:1717:LEU:N	2.51	0.43
1:G:469:ARG:HA	1:G:469:ARG:HD2	1.57	0.43
2:A:1353:LEU:HA	2:A:1356:PHE:HB3	2.00	0.43
2:A:875:THR:HG23	2:A:879:SER:HB3	2.00	0.43
1:B:63:LYS:HD3	1:B:125:ASN:HA	2.01	0.43
2:E:1364:GLU:OE1	2:E:1367:ARG:NH2	2.45	0.43
2:E:403:UNK:O	2:E:407:UNK:N	2.51	0.43
2:E:890:LYS:HA	2:E:890:LYS:HD3	1.91	0.43
2:A:403:UNK:O	2:A:407:UNK:N	2.51	0.43
2:A:795:MET:SD	2:A:795:MET:N	2.91	0.43
1:B:404:GLN:HA	1:B:408:PRO:HB3	2.00	0.43
2:E:739:GLN:NE2	2:E:794:ILE:O	2.51	0.43
1:F:485:ARG:HA	1:F:485:ARG:HD2	1.82	0.43
1:G:279:THR:O	1:G:283:ILE:N	2.49	0.43
2:A:752:ILE:HD12	2:A:765:LEU:HD22	2.01	0.43
1:B:1472:UNK:O	1:B:1476:UNK:N	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1718:THR:HG21	1:B:1770:LEU:HD13	2.00	0.43
1:B:1854:MET:HG3	1:B:1952:ALA:HB3	2.01	0.43
2:D:807:LYS:HE2	2:D:861:GLN:HE21	1.84	0.43
1:B:318:SER:OG	1:F:1259:UNK:O	2.25	0.43
1:G:1765:ARG:NH2	1:G:1767:GLU:OE2	2.52	0.43
1:G:1771:LEU:HD12	1:G:1771:LEU:HA	1.91	0.43
1:G:178:GLN:O	1:G:181:HIS:NE2	2.51	0.43
1:G:477:GLU:O	1:G:481:ASP:N	2.48	0.43
2:A:1148:HIS:NE2	2:A:1153:ASP:OD2	2.47	0.42
1:B:1895:ASN:HD21	1:B:1897:GLN:HA	1.84	0.42
1:F:1673:GLU:OE2	1:F:1676:MET:N	2.43	0.42
1:F:65:LEU:HD22	1:F:84:LEU:HB2	2.01	0.42
1:B:1214:UNK:O	1:B:1218:UNK:N	2.52	0.42
1:B:1745:LYS:HD3	1:B:1745:LYS:HA	1.79	0.42
1:B:259:THR:OG1	1:B:262:GLU:N	2.39	0.42
2:D:1148:HIS:NE2	2:D:1153:ASP:OD2	2.47	0.42
2:E:1126:ILE:HG23	2:E:1179:LEU:HA	2.00	0.42
2:E:1283:MET:SD	2:E:1283:MET:N	2.93	0.42
1:G:1694:ALA:O	1:G:1698:PHE:N	2.33	0.42
1:G:1863:ALA:HA	1:G:1866:PHE:HB3	2.00	0.42
2:A:949:GLU:O	2:A:953:VAL:N	2.41	0.42
1:B:104:LEU:HA	1:B:107:LYS:HB2	2.01	0.42
1:B:265:SER:OG	1:B:266:TYR:N	2.53	0.42
1:B:390:ASN:HA	1:B:393:LEU:HD12	2.01	0.42
3:C:1444:ASN:HA	3:C:1512:PHE:HE2	1.84	0.42
2:E:1307:THR:OG1	2:E:1310:GLU:OE2	2.33	0.42
1:G:1472:UNK:O	1:G:1476:UNK:N	2.52	0.42
1:G:1927:LEU:O	1:G:1930:SER:OG	2.38	0.42
1:G:259:THR:OG1	1:G:262:GLU:N	2.39	0.42
1:G:482:CYS:HA	1:G:486:LEU:HD12	2.00	0.42
1:G:3:ALA:N	1:G:9:LEU:O	2.39	0.42
2:A:1515:ARG:HD3	2:A:1515:ARG:HA	1.86	0.42
1:B:195:LEU:HA	1:B:198:LEU:HB2	2.01	0.42
1:B:38:ASN:HA	1:B:41:LEU:HG	2.00	0.42
1:B:927:UNK:O	1:B:931:UNK:N	2.52	0.42
2:D:820:ALA:O	2:D:863:THR:N	2.51	0.42
2:E:1313:ASP:HA	2:E:1316:VAL:HG12	2.02	0.42
1:F:491:GLU:O	1:F:494:THR:OG1	2.38	0.42
1:G:1854:MET:HG3	1:G:1952:ALA:HB3	2.01	0.42
1:G:4:TYR:OH	1:G:29:ILE:O	2.24	0.42
1:G:927:UNK:O	1:G:931:UNK:N	2.52	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1271:GLN:HE21	2:A:1274:ILE:HD13	1.85	0.42
1:B:1765:ARG:NH2	1:B:1767:GLU:OE2	2.52	0.42
1:B:825:UNK:N	1:B:836:UNK:O	2.53	0.42
2:D:919:LYS:HB3	2:D:919:LYS:HE3	1.88	0.42
2:E:1515:ARG:HA	2:E:1515:ARG:HD3	1.86	0.42
2:E:752:ILE:HD12	2:E:765:LEU:HD22	2.01	0.42
2:E:807:LYS:HE2	2:E:861:GLN:HE21	1.84	0.42
1:F:95:TYR:OH	1:F:111:GLU:OE1	2.35	0.42
1:F:1745:LYS:HD3	1:F:1745:LYS:HA	1.80	0.42
1:F:975:UNK:O	1:F:979:UNK:N	2.53	0.42
1:G:1895:ASN:HD21	1:G:1897:GLN:HA	1.84	0.42
3:H:1444:ASN:HA	3:H:1512:PHE:HE2	1.84	0.42
1:B:178:GLN:HA	1:B:181:HIS:CE1	2.54	0.42
2:D:1271:GLN:HE21	2:D:1274:ILE:HD13	1.85	0.42
2:D:1283:MET:SD	2:D:1283:MET:N	2.93	0.42
2:D:1364:GLU:OE1	2:D:1367:ARG:NH2	2.45	0.42
2:E:716:ASP:N	2:E:716:ASP:OD1	2.53	0.42
1:F:1863:ALA:HA	1:F:1866:PHE:HB3	2.00	0.42
1:F:255:LEU:HA	1:F:255:LEU:HD12	1.82	0.42
1:F:949:UNK:O	1:F:951:UNK:N	2.53	0.42
1:G:1312:UNK:HA	1:G:1565:UNK:HA	2.02	0.42
1:G:16:LEU:HA	1:G:19:VAL:HG22	2.02	0.42
1:G:949:UNK:O	1:G:951:UNK:N	2.53	0.42
2:A:1283:MET:SD	2:A:1283:MET:N	2.93	0.42
2:A:1312:VAL:O	2:A:1316:VAL:N	2.42	0.42
1:B:1872:GLN:HA	1:B:1875:VAL:HG22	2.02	0.42
1:B:491:GLU:O	1:B:494:THR:OG1	2.37	0.42
1:B:502:LEU:HA	1:B:502:LEU:HD23	1.92	0.42
1:B:65:LEU:HD11	1:B:83:VAL:HG13	2.01	0.42
1:F:1771:LEU:HD12	1:F:1771:LEU:HA	1.91	0.42
1:G:1716:ASN:OD1	1:G:1716:ASN:N	2.52	0.42
1:G:265:SER:OG	1:G:266:TYR:N	2.53	0.42
1:G:390:ASN:HA	1:G:393:LEU:HB2	2.00	0.42
1:G:38:ASN:HA	1:G:41:LEU:HG	2.00	0.42
1:G:63:LYS:HD3	1:G:125:ASN:HA	2.01	0.42
1:G:65:LEU:HD11	1:G:83:VAL:HG13	2.01	0.42
2:A:1313:ASP:HA	2:A:1316:VAL:HG12	2.02	0.42
2:A:526:VAL:O	2:A:530:ALA:N	2.51	0.42
2:A:807:LYS:HG3	2:A:861:GLN:HG2	2.02	0.42
1:B:16:LEU:HA	1:B:19:VAL:HG22	2.02	0.42
1:B:1905:ARG:CZ	1:B:1935:GLU:HG3	2.50	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HD22	1:B:84:LEU:HB2	2.01	0.42
1:B:728:UNK:HA	1:B:834:UNK:HA	2.01	0.42
1:B:975:UNK:O	1:B:979:UNK:N	2.53	0.42
2:D:873:ARG:NH2	2:D:882:ASN:OD1	2.53	0.42
2:E:807:LYS:HG3	2:E:861:GLN:HG2	2.02	0.42
1:F:1664:PHE:N	1:F:1803:THR:OG1	2.53	0.42
1:F:1895:ASN:HD21	1:F:1897:GLN:HA	1.84	0.42
1:F:195:LEU:HA	1:F:198:LEU:HB2	2.01	0.42
1:F:265:SER:OG	1:F:266:TYR:N	2.53	0.42
1:G:1685:LYS:HE2	1:G:1685:LYS:HB2	1.85	0.42
1:G:178:GLN:HA	1:G:181:HIS:CE1	2.54	0.42
1:G:728:UNK:HA	1:G:834:UNK:HA	2.01	0.42
3:I:1444:ASN:HA	3:I:1512:PHE:HE2	1.84	0.42
2:A:1702:UNK:O	2:A:1706:UNK:N	2.53	0.42
1:B:949:UNK:O	1:B:951:UNK:N	2.53	0.42
1:F:123:ILE:H	1:F:123:ILE:HG13	1.67	0.42
1:F:178:GLN:HA	1:F:181:HIS:CE1	2.54	0.42
1:F:404:GLN:HA	1:F:408:PRO:HB3	2.00	0.42
1:F:927:UNK:O	1:F:931:UNK:N	2.52	0.42
1:B:1694:ALA:O	1:B:1698:PHE:N	2.33	0.42
1:B:199:ILE:HG12	1:B:199:ILE:H	1.66	0.42
1:B:309:ARG:O	1:B:313:ALA:N	2.48	0.42
2:D:1111:PHE:CD2	2:D:1114:TYR:HB2	2.55	0.42
2:D:752:ILE:HD12	2:D:765:LEU:HD22	2.01	0.42
1:F:1564:UNK:HA	1:F:1655:ALA:H	1.84	0.42
1:F:1716:ASN:N	1:F:1716:ASN:OD1	2.52	0.42
1:G:156:LEU:HD21	1:G:502:LEU:HD12	2.01	0.42
1:G:975:UNK:O	1:G:979:UNK:N	2.53	0.42
1:B:1564:UNK:HA	1:B:1655:ALA:H	1.84	0.41
1:B:845:UNK:O	1:B:849:UNK:N	2.53	0.41
2:E:732:LEU:HD13	2:E:732:LEU:HA	1.82	0.41
1:G:1664:PHE:N	1:G:1803:THR:OG1	2.53	0.41
2:A:1138:LYS:HD2	2:A:1138:LYS:HA	1.85	0.41
2:A:1196:LYS:HA	2:A:1196:LYS:HD3	1.80	0.41
2:A:811:SER:OG	2:A:816:GLU:OE2	2.34	0.41
2:A:873:ARG:NH2	2:A:882:ASN:OD1	2.53	0.41
1:B:156:LEU:HD21	1:B:502:LEU:HD12	2.01	0.41
1:B:526:ARG:HG3	1:B:526:ARG:H	1.63	0.41
2:D:1247:SER:OG	2:D:1300:THR:N	2.48	0.41
2:E:820:ALA:O	2:E:863:THR:N	2.51	0.41
2:E:873:ARG:NH2	2:E:882:ASN:OD1	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:LEU:HD11	1:F:83:VAL:HG13	2.01	0.41
1:G:116:LEU:O	1:G:120:LYS:N	2.46	0.41
1:G:1872:GLN:HA	1:G:1875:VAL:HG22	2.02	0.41
1:G:503:ASP:N	1:G:527:VAL:O	2.47	0.41
2:A:1724:UNK:O	2:A:1726:UNK:N	2.53	0.41
2:A:405:UNK:O	2:A:409:UNK:N	2.53	0.41
1:B:1927:LEU:O	1:B:1930:SER:OG	2.37	0.41
1:B:255:LEU:HA	1:B:255:LEU:HD12	1.83	0.41
2:E:1254:VAL:O	2:E:1256:ALA:N	2.34	0.41
2:E:1418:VAL:HA	2:E:1419:PRO:HA	1.79	0.41
1:F:104:LEU:HA	1:F:107:LYS:HB2	2.01	0.41
1:F:279:THR:O	1:F:283:ILE:N	2.49	0.41
1:F:825:UNK:N	1:F:836:UNK:O	2.53	0.41
1:G:104:LEU:HA	1:G:107:LYS:HB2	2.01	0.41
1:G:1148:UNK:HA	1:G:1157:UNK:HA	2.03	0.41
1:G:1896:GLN:H	1:G:1899:VAL:HB	1.86	0.41
1:G:65:LEU:HD22	1:G:84:LEU:HB2	2.01	0.41
1:B:392:THR:HA	1:B:395:LYS:HB2	2.02	0.41
2:D:1393:ALA:O	2:D:1397:GLY:HA2	2.21	0.41
2:E:1724:UNK:O	2:E:1726:UNK:N	2.53	0.41
1:F:1927:LEU:O	1:F:1930:SER:OG	2.37	0.41
1:F:1854:MET:HG3	1:F:1952:ALA:HB3	2.01	0.41
1:F:845:UNK:O	1:F:849:UNK:N	2.53	0.41
1:G:1440:UNK:HA	1:G:1467:UNK:HA	2.02	0.41
1:G:601:UNK:O	1:G:605:UNK:N	2.54	0.41
1:G:677:UNK:O	1:G:679:UNK:N	2.54	0.41
2:A:807:LYS:HE2	2:A:861:GLN:HE21	1.84	0.41
2:A:884:ILE:HG21	2:A:943:LEU:HD13	2.02	0.41
2:A:908:LEU:HD11	2:A:926:LEU:HD21	2.03	0.41
2:D:1254:VAL:HG13	2:D:1255:SER:H	1.85	0.41
2:E:1271:GLN:HE21	2:E:1274:ILE:HD13	1.85	0.41
2:E:1702:UNK:O	2:E:1706:UNK:N	2.53	0.41
1:F:262:GLU:OE2	1:F:266:TYR:OH	2.24	0.41
1:F:677:UNK:O	1:F:679:UNK:N	2.54	0.41
1:F:728:UNK:HA	1:F:834:UNK:HA	2.01	0.41
1:G:1937:GLU:HG3	1:G:1937:GLU:H	1.78	0.41
1:G:217:GLU:OE2	1:G:221:ASN:ND2	2.54	0.41
1:G:825:UNK:N	1:G:836:UNK:O	2.53	0.41
2:A:1099:GLU:O	2:A:1101:SER:N	2.54	0.41
2:A:1759:UNK:O	2:A:1761:UNK:N	2.54	0.41
1:B:1685:LYS:HE2	1:B:1685:LYS:HB2	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:THR:OG1	1:B:271:THR:O	2.33	0.41
2:D:1313:ASP:HA	2:D:1316:VAL:HG12	2.02	0.41
2:D:1759:UNK:O	2:D:1761:UNK:N	2.54	0.41
2:D:676:LYS:NZ	2:D:767:ALA:HB2	2.36	0.41
2:D:908:LEU:HD11	2:D:926:LEU:HD21	2.03	0.41
2:E:1196:LYS:HA	2:E:1196:LYS:HD3	1.80	0.41
2:E:1326:ILE:HD12	2:E:1388:MET:HG2	2.00	0.41
2:E:1393:ALA:O	2:E:1397:GLY:HA2	2.21	0.41
2:E:370:UNK:O	2:E:374:UNK:N	2.54	0.41
2:E:824:LEU:HD13	2:E:824:LEU:HA	1.93	0.41
1:F:1872:GLN:HA	1:F:1875:VAL:HG22	2.02	0.41
1:F:601:UNK:O	1:F:605:UNK:N	2.54	0.41
1:B:1312:UNK:HA	1:B:1565:UNK:HA	2.02	0.41
1:B:1867:SER:OG	1:B:1867:SER:O	2.38	0.41
3:C:1475:GLU:O	3:C:1478:PRO:HD2	2.21	0.41
2:D:1099:GLU:O	2:D:1101:SER:N	2.54	0.41
2:D:1263:ASP:O	2:D:1267:ASP:N	2.54	0.41
2:E:1254:VAL:HG13	2:E:1255:SER:H	1.85	0.41
2:E:1516:ASP:OD2	2:E:1519:ILE:N	2.38	0.41
1:F:1884:TRP:N	1:F:1892:ASN:HD22	2.19	0.41
1:F:390:ASN:HA	1:F:393:LEU:HD12	2.01	0.41
1:G:1905:ARG:CZ	1:G:1935:GLU:HG3	2.50	0.41
2:A:1056:ILE:HA	2:A:1056:ILE:HD12	1.91	0.41
2:A:822:VAL:HG23	2:A:864:VAL:HA	2.03	0.41
1:B:1148:UNK:HA	1:B:1157:UNK:HA	2.03	0.41
1:B:1664:PHE:N	1:B:1803:THR:OG1	2.53	0.41
2:D:1236:LYS:HB2	2:D:1236:LYS:HE2	1.88	0.41
2:D:1702:UNK:O	2:D:1706:UNK:N	2.53	0.41
2:E:822:VAL:HG23	2:E:864:VAL:HA	2.03	0.41
1:F:1666:PHE:N	1:F:1805:ALA:O	2.53	0.41
1:F:187:LEU:HA	1:F:190:PHE:HB3	2.03	0.41
1:F:199:ILE:H	1:F:199:ILE:HG12	1.66	0.41
1:G:1884:TRP:N	1:G:1892:ASN:HD22	2.19	0.41
1:G:390:ASN:HA	1:G:393:LEU:HD12	2.01	0.41
1:G:491:GLU:O	1:G:494:THR:OG1	2.37	0.41
3:H:1464:GLU:HA	3:H:1467:LEU:HB2	2.03	0.41
2:A:1111:PHE:CD2	2:A:1114:TYR:HB2	2.55	0.41
2:A:676:LYS:NZ	2:A:767:ALA:HB2	2.36	0.41
2:A:820:ALA:N	2:A:861:GLN:O	2.51	0.41
1:B:1440:UNK:HA	1:B:1467:UNK:HA	2.02	0.41
1:B:217:GLU:OE2	1:B:221:ASN:ND2	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1724:UNK:O	2:D:1726:UNK:N	2.53	0.41
2:D:383:UNK:O	2:D:387:UNK:N	2.54	0.41
2:D:405:UNK:O	2:D:409:UNK:N	2.53	0.41
2:D:807:LYS:HG3	2:D:861:GLN:HG2	2.02	0.41
2:E:1759:UNK:O	2:E:1761:UNK:N	2.54	0.41
1:F:63:LYS:HD3	1:F:125:ASN:HA	2.01	0.41
1:F:1312:UNK:HA	1:F:1565:UNK:HA	2.02	0.41
1:F:1905:ARG:CZ	1:F:1935:GLU:HG3	2.50	0.41
1:G:1564:UNK:HA	1:G:1655:ALA:H	1.84	0.41
1:G:2033:THR:O	1:G:2037:PRO:N	2.54	0.41
1:G:88:LEU:O	1:G:92:GLU:N	2.53	0.41
1:B:515:LEU:HA	1:B:515:LEU:HD12	1.83	0.41
2:D:822:VAL:HG23	2:D:864:VAL:HA	2.03	0.41
2:E:1099:GLU:O	2:E:1101:SER:N	2.54	0.41
1:F:16:LEU:HA	1:F:19:VAL:HG22	2.02	0.41
1:F:286:THR:HG21	1:F:292:PHE:HD1	1.86	0.41
1:F:88:LEU:O	1:F:92:GLU:N	2.53	0.41
1:G:1309:UNK:O	1:G:1616:VAL:N	2.54	0.41
1:G:392:THR:HA	1:G:395:LYS:HB2	2.02	0.41
1:G:845:UNK:O	1:G:849:UNK:N	2.53	0.41
3:I:1475:GLU:O	3:I:1478:PRO:HD2	2.21	0.41
2:A:1393:ALA:O	2:A:1397:GLY:HA2	2.21	0.41
1:B:1716:ASN:OD1	1:B:1716:ASN:N	2.52	0.41
1:B:1770:LEU:O	1:B:1772:SER:N	2.54	0.41
1:B:1896:GLN:H	1:B:1899:VAL:HB	1.86	0.41
1:B:2033:THR:O	1:B:2037:PRO:N	2.54	0.41
2:D:1234:MET:SD	2:D:1239:HIS:NE2	2.94	0.41
2:D:373:UNK:O	2:D:377:UNK:N	2.54	0.41
2:D:884:ILE:HG21	2:D:943:LEU:HD13	2.02	0.41
2:E:1111:PHE:CD2	2:E:1114:TYR:HB2	2.55	0.41
2:E:1420:ALA:HA	2:E:1421:PRO:HD3	1.96	0.41
2:E:884:ILE:HG21	2:E:943:LEU:HD13	2.02	0.41
1:G:1887:GLU:HB2	1:G:1890:ASN:HB3	2.03	0.41
1:G:286:THR:HG21	1:G:292:PHE:HD1	1.86	0.41
1:G:292:PHE:O	1:G:296:VAL:HG23	2.21	0.41
2:A:1094:GLU:HG2	2:A:1098:LEU:HD23	2.03	0.40
1:B:158:ALA:HB3	1:B:270:ALA:HA	2.03	0.40
1:B:677:UNK:O	1:B:679:UNK:N	2.54	0.40
2:D:1094:GLU:HG2	2:D:1098:LEU:HD23	2.04	0.40
2:D:862:LEU:HD13	2:D:862:LEU:HA	1.89	0.40
2:E:676:LYS:NZ	2:E:767:ALA:HB2	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:908:LEU:HD11	2:E:926:LEU:HD21	2.03	0.40
2:E:919:LYS:HB3	2:E:919:LYS:HE3	1.87	0.40
1:F:4:TYR:OH	1:F:29:ILE:O	2.24	0.40
1:G:1666:PHE:N	1:G:1805:ALA:O	2.54	0.40
1:G:195:LEU:HA	1:G:198:LEU:HB2	2.01	0.40
2:A:1263:ASP:O	2:A:1267:ASP:N	2.54	0.40
1:B:1309:UNK:O	1:B:1616:VAL:N	2.54	0.40
1:B:1695:ASP:OD2	1:B:1706:ILE:N	2.54	0.40
1:B:286:THR:HG21	1:B:292:PHE:HD1	1.86	0.40
1:B:79:GLN:H	1:B:79:GLN:HG3	1.73	0.40
2:D:1421:PRO:HD2	2:D:1423:LYS:NZ	2.36	0.40
2:D:526:VAL:O	2:D:530:ALA:N	2.51	0.40
2:D:716:ASP:OD1	2:D:716:ASP:N	2.53	0.40
2:E:383:UNK:O	2:E:387:UNK:N	2.54	0.40
1:F:116:LEU:O	1:F:120:LYS:N	2.46	0.40
1:F:1896:GLN:H	1:F:1899:VAL:HB	1.86	0.40
1:F:158:ALA:HB3	1:F:270:ALA:HA	2.03	0.40
1:G:1695:ASP:OD2	1:G:1706:ILE:N	2.54	0.40
1:G:237:SER:HA	1:G:240:LEU:HB3	2.03	0.40
1:B:1884:TRP:N	1:B:1892:ASN:HD22	2.19	0.40
1:B:292:PHE:O	1:B:296:VAL:HG23	2.21	0.40
1:B:66:GLY:O	1:B:69:SER:OG	2.34	0.40
3:C:1464:GLU:HG2	3:C:1464:GLU:H	1.64	0.40
2:E:1234:MET:SD	2:E:1239:HIS:NE2	2.94	0.40
1:F:1440:UNK:HA	1:F:1467:UNK:HA	2.02	0.40
2:A:1254:VAL:HG13	2:A:1255:SER:H	1.85	0.40
2:A:373:UNK:O	2:A:377:UNK:N	2.55	0.40
1:B:1771:LEU:HA	1:B:1771:LEU:HD12	1.91	0.40
1:B:1666:PHE:N	1:B:1805:ALA:O	2.53	0.40
1:B:1858:ASN:ND2	1:B:1859:PRO:O	2.55	0.40
1:B:309:ARG:HB3	1:B:435:ALA:HB1	2.04	0.40
3:C:1460:LYS:HE3	3:C:1460:LYS:HB3	1.88	0.40
2:D:1196:LYS:HD3	2:D:1196:LYS:HA	1.80	0.40
1:F:1148:UNK:HA	1:F:1157:UNK:HA	2.02	0.40
1:F:1695:ASP:OD2	1:F:1706:ILE:N	2.54	0.40
1:F:1809:LEU:HD23	1:F:1812:TYR:HD2	1.87	0.40
1:F:1887:GLU:HB2	1:F:1890:ASN:HB3	2.03	0.40
1:G:187:LEU:HA	1:G:190:PHE:HB3	2.03	0.40
1:G:309:ARG:HB3	1:G:435:ALA:HB1	2.04	0.40
2:A:370:UNK:O	2:A:374:UNK:N	2.54	0.40
2:A:383:UNK:O	2:A:387:UNK:N	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:807:LYS:NZ	2:A:811:SER:OG	2.52	0.40
1:B:601:UNK:O	1:B:605:UNK:N	2.54	0.40
2:D:820:ALA:N	2:D:861:GLN:O	2.51	0.40
2:E:1192:GLY:HA3	2:E:1193:TRP:CE3	2.56	0.40
2:E:1394:LEU:HA	2:E:1394:LEU:HD23	1.84	0.40
2:E:624:LYS:O	2:E:628:SER:N	2.54	0.40
2:E:746:GLU:HA	2:E:749:ILE:HG22	2.04	0.40
1:F:2033:THR:O	1:F:2037:PRO:N	2.54	0.40
1:F:217:GLU:OE2	1:F:221:ASN:ND2	2.54	0.40
1:F:337:PRO:O	1:F:380:SER:OG	2.40	0.40
1:G:1423:UNK:HA	1:G:1449:UNK:HA	2.04	0.40
1:G:1770:LEU:O	1:G:1772:SER:N	2.54	0.40
1:G:1809:LEU:HD23	1:G:1812:TYR:HD2	1.87	0.40
1:G:255:LEU:HD12	1:G:255:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	986/2051 (48%)	735 (74%)	209 (21%)	42 (4%)	3	28
1	F	986/2051 (48%)	735 (74%)	210 (21%)	41 (4%)	3	28
1	G	986/2051 (48%)	735 (74%)	210 (21%)	41 (4%)	3	28
2	A	879/1887 (47%)	629 (72%)	216 (25%)	34 (4%)	3	29
2	D	879/1887 (47%)	628 (71%)	217 (25%)	34 (4%)	3	29
2	E	879/1887 (47%)	628 (71%)	217 (25%)	34 (4%)	3	29
3	C	69/71 (97%)	48 (70%)	21 (30%)	0	100	100
3	H	69/71 (97%)	48 (70%)	21 (30%)	0	100	100
3	I	69/71 (97%)	49 (71%)	20 (29%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5802/12027 (48%)	4235 (73%)	1341 (23%)	226 (4%)	6	29

All (226) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	558	ASN
1	B	567	PRO
1	B	1618	PRO
1	B	1632	ILE
1	B	1862	VAL
1	B	1925	ILE
1	B	1955	PRO
1	B	1957	PRO
1	B	1968	PRO
1	B	1996	ILE
2	A	589	ASP
2	A	617	PRO
2	A	636	PRO
2	A	644	THR
2	A	645	PRO
2	A	787	LYS
2	A	1158	PRO
1	F	558	ASN
1	F	567	PRO
1	F	1618	PRO
1	F	1632	ILE
1	F	1862	VAL
1	F	1925	ILE
1	F	1955	PRO
1	F	1957	PRO
1	F	1968	PRO
1	F	1996	ILE
2	D	589	ASP
2	D	617	PRO
2	D	636	PRO
2	D	644	THR
2	D	645	PRO
2	D	787	LYS
2	D	1158	PRO
1	G	558	ASN
1	G	567	PRO
1	G	1618	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	1632	ILE
1	G	1862	VAL
1	G	1925	ILE
1	G	1955	PRO
1	G	1957	PRO
1	G	1968	PRO
1	G	1996	ILE
2	E	589	ASP
2	E	617	PRO
2	E	636	PRO
2	E	644	THR
2	E	645	PRO
2	E	787	LYS
2	E	1158	PRO
1	B	547	ILE
1	B	550	VAL
1	B	566	HIS
1	B	1633	ASN
1	B	1638	ILE
1	B	1716	ASN
1	B	1924	ILE
1	B	1956	ARG
1	B	1977	HIS
1	B	1979	THR
1	B	2029	VAL
2	A	525	TYR
2	A	526	VAL
2	A	552	LYS
2	A	553	ALA
2	A	614	ALA
2	A	646	ALA
2	A	667	ALA
2	A	1092	LYS
2	A	1100	HIS
2	A	1159	GLU
2	A	1255	SER
1	F	547	ILE
1	F	550	VAL
1	F	566	HIS
1	F	1633	ASN
1	F	1638	ILE
1	F	1716	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	1924	ILE
1	F	1956	ARG
1	F	1977	HIS
1	F	1979	THR
1	F	2029	VAL
2	D	525	TYR
2	D	526	VAL
2	D	552	LYS
2	D	553	ALA
2	D	614	ALA
2	D	646	ALA
2	D	667	ALA
2	D	1092	LYS
2	D	1100	HIS
2	D	1159	GLU
2	D	1255	SER
1	G	547	ILE
1	G	550	VAL
1	G	566	HIS
1	G	1633	ASN
1	G	1638	ILE
1	G	1716	ASN
1	G	1924	ILE
1	G	1956	ARG
1	G	1977	HIS
1	G	1979	THR
1	G	2029	VAL
2	E	525	TYR
2	E	526	VAL
2	E	552	LYS
2	E	553	ALA
2	E	614	ALA
2	E	646	ALA
2	E	667	ALA
2	E	1092	LYS
2	E	1100	HIS
2	E	1159	GLU
2	E	1255	SER
1	B	447	ASN
1	B	1962	ARG
1	B	1965	ALA
1	B	1966	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2011	ILE
1	B	2017	LYS
2	A	603	ASP
2	A	608	ASP
2	A	618	ASN
2	A	648	ASP
2	A	1047	LEU
2	A	1080	THR
1	F	447	ASN
1	F	1962	ARG
1	F	1965	ALA
1	F	1966	CYS
1	F	2011	ILE
1	F	2017	LYS
1	F	2022	THR
2	D	603	ASP
2	D	608	ASP
2	D	618	ASN
2	D	648	ASP
2	D	1047	LEU
2	D	1080	THR
1	G	447	ASN
1	G	1962	ARG
1	G	1965	ALA
1	G	1966	CYS
1	G	2011	ILE
1	G	2017	LYS
1	G	2022	THR
2	E	603	ASP
2	E	608	ASP
2	E	618	ASN
2	E	648	ASP
2	E	1047	LEU
2	E	1080	THR
1	B	1631	MET
1	B	1734	SER
1	B	1959	LYS
1	B	2000	ASN
1	B	2014	LEU
1	B	2022	THR
2	A	628	SER
2	A	1083	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	1111	PHE
1	F	1631	MET
1	F	1734	SER
1	F	1959	LYS
1	F	2000	ASN
1	F	2014	LEU
2	D	628	SER
2	D	1083	PRO
2	D	1111	PHE
1	G	1631	MET
1	G	1734	SER
1	G	1959	LYS
1	G	2000	ASN
1	G	2014	LEU
2	E	628	SER
2	E	1083	PRO
2	E	1111	PHE
1	B	1650	VAL
1	B	1753	LYS
1	B	1918	LYS
2	A	595	GLN
2	A	609	SER
2	A	611	LYS
1	F	1650	VAL
1	F	1753	LYS
1	F	1918	LYS
2	D	595	GLN
2	D	609	SER
2	D	611	LYS
1	G	1650	VAL
1	G	1753	LYS
1	G	1918	LYS
2	E	595	GLN
2	E	609	SER
2	E	611	LYS
1	B	1976	PHE
1	B	2020	GLN
1	B	2021	VAL
1	F	1976	PHE
1	F	2021	VAL
1	G	1976	PHE
1	G	2021	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	42	PRO
1	B	1944	ILE
1	F	1944	ILE
1	G	1944	ILE
1	F	42	PRO
1	G	42	PRO
2	A	1326	ILE
2	D	1326	ILE
2	E	1326	ILE
1	B	1648	VAL
2	A	1071	PRO
2	A	1107	GLU
1	F	1648	VAL
2	D	1071	PRO
2	D	1107	GLU
1	G	1648	VAL
2	E	613	VAL
2	E	1071	PRO
2	E	1107	GLU
2	A	613	VAL
2	D	613	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	690/877 (79%)	682 (99%)	8 (1%)	74	87
1	F	690/877 (79%)	682 (99%)	8 (1%)	74	87
1	G	690/877 (79%)	682 (99%)	8 (1%)	74	87
2	A	610/845 (72%)	596 (98%)	14 (2%)	53	76
2	D	610/845 (72%)	596 (98%)	14 (2%)	53	76
2	E	610/845 (72%)	596 (98%)	14 (2%)	53	76
3	C	64/64 (100%)	63 (98%)	1 (2%)	65	83
3	H	64/64 (100%)	63 (98%)	1 (2%)	65	83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	64/64 (100%)	63 (98%)	1 (2%)	65	83
All	All	4092/5358 (76%)	4023 (98%)	69 (2%)	66	82

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	CYS
1	B	96	LEU
1	B	115	THR
1	B	202	THR
1	B	518	ARG
1	B	1682	LYS
1	B	1738	PHE
1	B	1768	LYS
2	A	685	LYS
2	A	707	THR
2	A	757	LYS
2	A	863	THR
2	A	906	LEU
2	A	925	ASP
2	A	1191	THR
2	A	1246	CYS
2	A	1273	ASP
2	A	1305	CYS
2	A	1309	VAL
2	A	1329	VAL
2	A	1398	VAL
2	A	1406	MET
3	C	1478	PRO
1	F	94	CYS
1	F	96	LEU
1	F	115	THR
1	F	202	THR
1	F	518	ARG
1	F	1682	LYS
1	F	1738	PHE
1	F	1768	LYS
2	D	685	LYS
2	D	707	THR
2	D	757	LYS
2	D	863	THR
2	D	906	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	925	ASP
2	D	1191	THR
2	D	1246	CYS
2	D	1273	ASP
2	D	1305	CYS
2	D	1309	VAL
2	D	1329	VAL
2	D	1398	VAL
2	D	1406	MET
3	H	1478	PRO
1	G	94	CYS
1	G	96	LEU
1	G	115	THR
1	G	202	THR
1	G	518	ARG
1	G	1682	LYS
1	G	1738	PHE
1	G	1768	LYS
2	E	685	LYS
2	E	707	THR
2	E	757	LYS
2	E	863	THR
2	E	906	LEU
2	E	925	ASP
2	E	1191	THR
2	E	1246	CYS
2	E	1273	ASP
2	E	1305	CYS
2	E	1309	VAL
2	E	1329	VAL
2	E	1398	VAL
2	E	1406	MET
3	I	1478	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	ASN
1	B	110	GLN
1	B	155	GLN
1	B	178	GLN
1	B	221	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	245	GLN
1	B	350	GLN
1	B	390	ASN
1	B	1688	GLN
1	B	1692	ASN
1	B	1892	ASN
1	B	1896	GLN
2	A	758	ASN
2	A	792	HIS
2	A	1271	GLN
2	A	1433	HIS
3	C	1495	ASN
1	F	93	ASN
1	F	110	GLN
1	F	155	GLN
1	F	178	GLN
1	F	221	ASN
1	F	245	GLN
1	F	350	GLN
1	F	390	ASN
1	F	1688	GLN
1	F	1692	ASN
1	F	1892	ASN
1	F	1896	GLN
2	D	758	ASN
2	D	792	HIS
2	D	1271	GLN
2	D	1433	HIS
3	H	1495	ASN
1	G	93	ASN
1	G	110	GLN
1	G	155	GLN
1	G	178	GLN
1	G	221	ASN
1	G	245	GLN
1	G	350	GLN
1	G	390	ASN
1	G	1688	GLN
1	G	1692	ASN
1	G	1892	ASN
1	G	1896	GLN
2	E	758	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	792	HIS
2	E	1271	GLN
2	E	1433	HIS
3	I	1495	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.